(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
7 September 2001 (07.09.2001)

PCT

(10) International Publication Number
WO 01/65415 A2

(51) International Patent Classification[7]: G06F 17/30

(21) International Application Number: PCT/US01/06443

(22) International Filing Date: 28 February 2001 (28.02.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/186,156 29 February 2000 (29.02.2000) US

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(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

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— *without international search report and to be republished upon receipt of that report*

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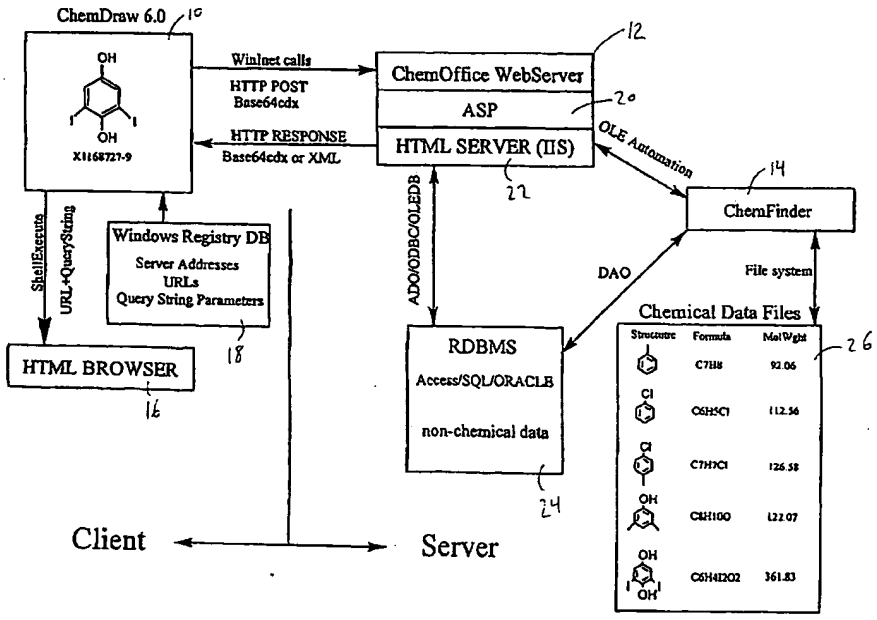
(54) Title: MANAGING CHEMICAL INFORMATION AND COMMERCE



(57) Abstract: A description of a chemical substance is acquired and a user's selection of a user interface menu item is detected. The user interface menu item pertains to a Web server having access to data for chemical substances. Based on the detection, a request is submitted to the Web server for information based on the description of the chemical substance. A response is received from the Web server that includes data pertaining to the chemical substance. Ouput data is derived from the data pertaining to the chemical substance.

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MANAGING CHEMICAL INFORMATION AND COMMERCE

This application claims the benefit of United States Provisional Application Serial No. 60/186,156 entitled "MANAGING CHEMICAL PRODUCT COMMERCE", filed on February 29, 2000, which is incorporated herein by reference.

Background of the Invention

This application relates to managing chemical information and commerce.

A chemistry oriented application program such as a chemical drawing program allows chemical information to be handled as computer data by a computer. A chemical drawing program typically allows a user to cause chemical structural information and chemical reaction information to be displayed on a computer screen and printed out on a computer printer. If a user has chemical information in the application program that is relevant to another application program, the user typically can use the cut and paste capabilities of the application program to copy the relevant information to the other application program. If one of the application programs is a Web browser interacting with a Web server, the user typically can use the cut and paste capabilities to share information between the Web browser and the other application program, and can thereby, in a limited way, share information between the Web server and the other application program. However, existing chemically oriented application programs provide inadequate abilities to access chemical information that is stored in different formats or in remote locations.

Summary of the Invention

Methods and systems are provided for managing chemical information and commerce. In particular, an external query capability allows a chemistry oriented application program to query an external entity such as a chemical information external database using

the Hypertext Transfer Protocol ("HTTP"), to produce information management and commerce management results not otherwise realizable by the application program.

Different aspects of the invention allow one or more of the following. An application program having chemical information can submit that information in a query to a remote chemical database and receive and incorporate a response from the database, without requiring the user to run or exercise another application program such as a Web browser. A user can provide chemical information in one form (e.g., structural) to an application program which can submit the information to another entity such as a remote database in a different form (e.g., textual) that is meaningful to the other entity, and that can lead to retrieval of information that is useful to the user. The capabilities of a chemistry oriented software tool can be linked to, and thereby applied to, a remote organized set of chemical information to produce analytical and commercial results such as reports and purchasing lists based on the remote organized set of chemical information.

Other features and advantages will become apparent from the following description, including the drawings, and from the claims.

Brief Description of the Drawings

Fig. 1 is a block diagram of a computer-based system.

Figs. 2-11, 16 are illustrations of output displays that may be produced by the computer based system.

Figs. 12A-15 are illustrations of data forms that may be used in the computer based system.

Detailed Description

A chemistry oriented application program has an external query capability that allows the program to query an external entity such as a chemical information external database.

Fig. 1 illustrates an example system in which a chemical drawing application program 10 (in this example, ChemDraw 6.0, provided by CambridgeSoft Corporation of Cambridge, Massachusetts) serves as the application program and uses the external query capability to acquire information via HTTP from a Web server 12 (in this example, ChemOffice WebServer, provided by CambridgeSoft Corporation of Cambridge, Massachusetts) linked to a chemical information database 14 (in this example, ChemFinder, provided by CambridgeSoft Corporation of Cambridge, Massachusetts). Although these particular chemistry oriented programs are provided to illustrate the present invention, other applications programs, Web servers, databases, and other programs may be used as well or instead.

In the example system, which is a Microsoft Windows implementation using ChemDraw, ChemDraw can, if necessary, invoke a Web browser 16 (e.g., see the third and fourth examples below) and can retrieve information including server addresses, uniform resource locators (URLs), and query string parameters from a Windows registry database ("Windows registry") 18. ChemDraw can use WinInet calls to post HTTP requests to the ChemOffice Webserver, and receives responses in HTTP form. WinInet, which is supplied as part of the Windows operating system, is a set of functions (also known as calls, procedures, and subroutines) in an Internet application programming interface (API) that may be implemented as dynamic link library file (DLL). A DLL provides a library of functions that applications link to and call as regular function calls.

The ChemOffice WebServer uses Active Server Pages ("ASP") software 20 and Hypertext Markup Language (HTML) server software known as Internet Information Server ("IIS") 22 to interact with ChemFinder via Object Linking and Embedding (OLE) Automation, and with a relational database management system ("RDBMS") 24. (Other interaction mechanisms may be used in place of or in addition to OLE Automation.) Web pages managed by ChemOffice WebServer may be formatted according to HTML or XML (Extensible Markup Language). Additionally, Web pages may be formatted as, for example, active server page text files ("ASP files") compatible with the ASP software. An ASP file may rely on a combination of HTML or XML and a scripting language such as VBScript or JavaScript.

The interaction with the RDBMS is implemented using one or more data access technologies such as Open Database Connectivity (ODBC), Active Data Objects (ADO), and OLEDB. ODBC is a standard for accessing different database systems from a high level programming language application, and enables applications to submit statements to ODBC using structured query language (SQL), which statements are then translated to the particular SQL commands that are used by the specific underlying database product.

The RDBMS includes non-chemical data such as substance prices. ChemFinder is able to retrieve chemical information such as chemical structure data ("chemical structure"), chemical formulas, and molecular weights from chemical data files 26, and interacts with the RDBMS using, e.g., ADO technology. According to ADO, data from a database is mapped into active data objects which perform the actual queries to the database. This approach provides substantial abstraction by limiting exposure only to the resultant objects.

ChemDraw communicates with an external chemical database server as now described with reference to multiple examples including an example illustrating how ChemDraw may be used to purchase chemicals online at the Available Chemicals Xchange web site (ChemACX.com). ChemDraw can initiate a database query based on either a chemical structure drawing or a simple text string. (Other application programs may use other data formats.) The response provided by the chemical database server can be a simple text response, a chemical structure, or a complex record set containing a combination of chemical and non-chemical data. The process by which ChemDraw handles a query differs slightly depending on the request/response method that is available.

In a first example, a chemical structure drawing is used to retrieve a plain text response. Using ChemDraw, the user creates a drawing of a molecule which is stored as chemical structure by ChemDraw in a native binary format known as cdx.

When the user selects "Look up ACX number from structure" from an online menu 40 (Figs. 2-3), which is a pulldown menu in ChemDraw, ChemDraw converts the chemical structure data from the cdx format to an ASCII text representation. The cdx-to-ASCII conversion is accomplished via a base64 encoding process with a subsequent URL encoding for safe transport over the HTTP protocol. Base64 is an encoding scheme defined by the Multipurpose Internet Mail Extensions (MIME) standard, and is defined to provide robustness to binary data that is expected to confront transformations while traversing the Internet. Base64 encoding converts binary data into alphanumeric characters. For example, binary data such as "110110001011010100000101" may be encoded as textual data "sLUF" which may be transmitted across the Internet.

ChemDraw uses configuration information stored in the Windows registry database to derive a target URL, i.e., a URL pointing to a remote chemical database server. Using the URL derived from the registry information and the URL encoded ASCII text representation of the chemical structure drawn by the user, ChemDraw uses WinInet to post an HTTP request. The converted chemical structure data is passed in the body of the HTTP request.

The remote chemical database server responds with a comma delimited text string containing one or more ACX numbers (e.g., ACX number X1069636-5 shown in Fig. 4) corresponding to the chemical structure drawn by the user. (ACX numbers are product identifiers described in two commonly assigned co-pending applications filed May 5, 2000: 09/565,085 entitled "DERIVING PRODUCT INFORMATION", and 09/565,810 entitled "MANAGING PRODUCT INFORMATION", which applications are incorporated herein by reference.)

ChemDraw captures the server's response by reading the HTTP response.

As shown by example in Fig. 5, the ACX numbers received from the server are displayed by ChemDraw on the ChemDraw canvas in a text box displayed near, e.g., immediately below, the user's chemical structure drawing.

In a second example, a plain text input value is used to retrieve a chemical structure drawing. In particular, a reverse version of the first example above can be accomplished by providing a valid ACX number and retrieving the corresponding chemical structure. In this example, the user selects "Lookup structure from the ACX number" in the ChemDraw 6.0 online menu.

A dialog box shown by example in Fig. 6 opens and prompts the user to enter an ACX number.

ChemDraw retrieves target URL information from the Windows registry and builds an HTTP request. In this case, the payload of the HTTP request is a string containing the ACX number, which is appended to the URL as a query string. The HTTP response returned by the remote server contains a URL encoded base64 text representation of a chemical structure. ChemDraw decodes the text representation and displays the structure on its canvas as a native ChemDraw picture shown by example in Fig. 7.

In a third example, an external HTML browser session is initiated with a remote server. Although ChemDraw is able to access remote servers by directly managing HTTP calls, ChemDraw can also delegate interactions with the server to an external HTML browser. A user selects a "Browse ChemStore.Com" online menu item in ChemDraw, which causes the default HMTL browser to be launched on the user's computer and directed to load a Web page from ChemStore.com as shown by example in Fig. 8.

ChemDraw proceeds in the third example as follows. ChemDraw builds a URL from configurable data stored in the Windows registry. ChemDraw issues a call to ShellExecute with the target URL as a parameter, which causes the user's default browser to open and load the page specified by the URL. (In Microsoft Windows, the ShellExecute function either launches the specified application program, or, if the program is already executing, makes the program the current window.)

Complex URLs corresponding to user specific server pages can be built by incorporating data received from previous queries using techniques described in the first and second examples above. For example, a specific page from a chemical supplier's catalog can be retrieved based on a structure of a molecule drawn by the user.

In a fourth example, a user accomplishes online purchasing of chemicals by starting from ChemDraw. The first and second examples above illustrate how ChemDraw can send or receive a chemical structure or text data to or from a remote chemical database server and display the results directly in ChemDraw's drawing area. When the results of a query are expected to be lengthy or complex, ChemDraw causes a standard HTML browser to handle the display instead.

In this example, chemicals are purchased online from ChemACX.com. As described in the first example above, the user draws a molecule and selects the "Lookup suppliers from ChemACX.com" online menu item.

The chemical structure drawn by the user is used in this example to identify the substance for which purchasing information is to be fetched. Thus, the procedure is as described in the first example above, except that the value returned by the server is a substance identifier that is not meaningful to the end user, and therefore is not displayed, but is used as an intermediate value for querying a Web based catalog.

Specifically, the substance identifier is posted to a remote server to obtain the desired purchasing information. The requested result set is to be displayed in an external browser window. Accordingly, ChemDraw uses techniques described above in the third example to build a URL pointing the specific catalog page at ChemACX.Com which contains information about the desired substance. This URL is built from server target information stored in the Windows registry database and from the unique substance identifier fetched from the server in the initial step described above.

ChemDraw opens the user's default external browser and automatically causes the browser to load the appropriate catalog page. The user can use the browser to navigate the

available purchasing information and initiate the online ordering process from within the browser.

In a specific implementation in which the user is presented with a list of suppliers and prices in a Web browser window, the user can then check off the supplier and desired quantity, which causes a corresponding shopping cart construct to be created, ready for submission for purchase completion.

The online menu may also be configured to retrieve other pieces of data based on a selected structure, such as specific compound identification numbers from specific manufacturers.

Figs. 12A-16 illustrate a specific example of data transformations referenced above, with respect to an example interaction when a user draws a structure and selects the "Find ACX Numbers from Structure" online menu item. Figs. 12A-12B illustrate a chemical structure and its corresponding binary CDX form. Fig. 13 illustrates the base64 encoded form corresponding to Figs. 12A-12B. Fig. 14 illustrates the encoded request corresponding to Fig. 13. Fig. 15 illustrates the response from the server corresponding to Fig. 14. Fig. 16 illustrates a display provided to the user corresponding to Fig. 15.

Figs. 9-11 illustrate examples of other pages that may be retrieved by selection of, respectively, the "CambridgeSoft Home Page", "CS ChemDraw Technical Support", and "Register Online" online menu items shown in Figs. 2-3.

All, or a portion, of the procedures described above may be implemented in hardware or software, or a combination of both. In at least some cases, it is advantageous if the technique is implemented in computer programs executing on one or more programmable computers, such as a personal computer running or able to run an operating system such as

Unix, Linux, Microsoft Windows 95, 98, 2000, or NT, or Macintosh OS, that each include a processor, a storage medium readable by the processor (including volatile and non-volatile memory and/or storage elements), at least one input device such as a keyboard, and at least one output device. Program code is applied to data entered using the input device to perform the technique described above and to generate output information. The output information is applied to one or more output devices such as a display screen of the computer.

In at least some cases, it is advantageous if each program is implemented in a high level procedural or object-oriented programming language such as Perl, C, C++, or Java to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

In at least some cases, it is advantageous if each such computer program is stored on a storage medium or device, such as ROM or optical or magnetic disc, that is readable by a general or special purpose programmable computer for configuring and operating the computer when the storage medium or device is read by the computer to perform the procedures described in this document. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner.

Other embodiments are within the scope of the following claims. For example, a more general range of services may be provided. A query may be performed on local or remote databases, and may be used in the derivation of a non-exact query or a non-structural query. For instance, in the case of ChemDraw which provides property prediction facilities,

such facilities may be used to predict physical characteristics of a molecule of interest, and local or remote databases may be searched for substances having similar properties. The online menu may be used in another application program such as a spreadsheet program. For instance, in the case of the spreadsheet program, the program may store a shopping list of chemical products, and the online menu may include a selectable item for retrieving price information for each listed product from a remote chemical information database and embedding the retrieved price information in the shopping list.

What is claimed is:

1. A method for use in managing chemical information, comprising:

acquiring a description of a chemical substance;

detecting a user's selection of a user interface menu item pertaining to a Web server having access to data for chemical substances;

based on the detection, submitting, to the Web server, a request for information based on the description of the chemical substance;

receiving a response from the Web server, the response including data pertaining to the chemical substance; and

deriving output data from the data pertaining to the chemical substance.

2. The method of claim 1, wherein the description of the chemical substance includes a structural description of the chemical substance.

3. The method of claim 1, wherein the description of the chemical substance includes a textual description of the textual substance.

4. The method of claim 1, wherein the output data includes structural output data.

5. The method of claim 1, wherein the output data includes textual output data.

6. The method of claim 1, wherein the output data includes commercial product data.

7. The method of claim 1, wherein the user interface item is provided by a chemistry oriented application program.

8. The method of claim 7, wherein the chemistry oriented application program includes a chemical drawing program.

9. The method of claim 1, further comprising

formatting at least a portion of the request for information according to the HTTP protocol.

10. The method of claim 1, further comprising

decoding at least a portion of the response from the Web server according to the HTTP protocol.

11. The method of claim 1, further comprising

presenting a user interface window that includes a display corresponding to the description of the chemical substance and another display derived from the output data.

12. The method of claim 1, further comprising

causing a new Web browser window to be displayed; and

causing a display derived from the output data to be displayed in the new Web browser window.

13. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to manage chemical information, the instructions causing the system to:

acquire a description of a chemical substance;

detect a user's selection of a user interface menu item pertaining to a Web server having access to data for chemical substances;

based on the detection, submit, to the Web server, a request for information based on the description of the chemical substance;

receive a response from the Web server, the response including data pertaining to the chemical substance; and

derive output data from the data pertaining to the chemical substance.

14. A system for use in managing chemical information, comprising:

a Web server having access to data for chemical substances; and

a chemistry oriented application program providing a user interface menu item linked to the Web server.

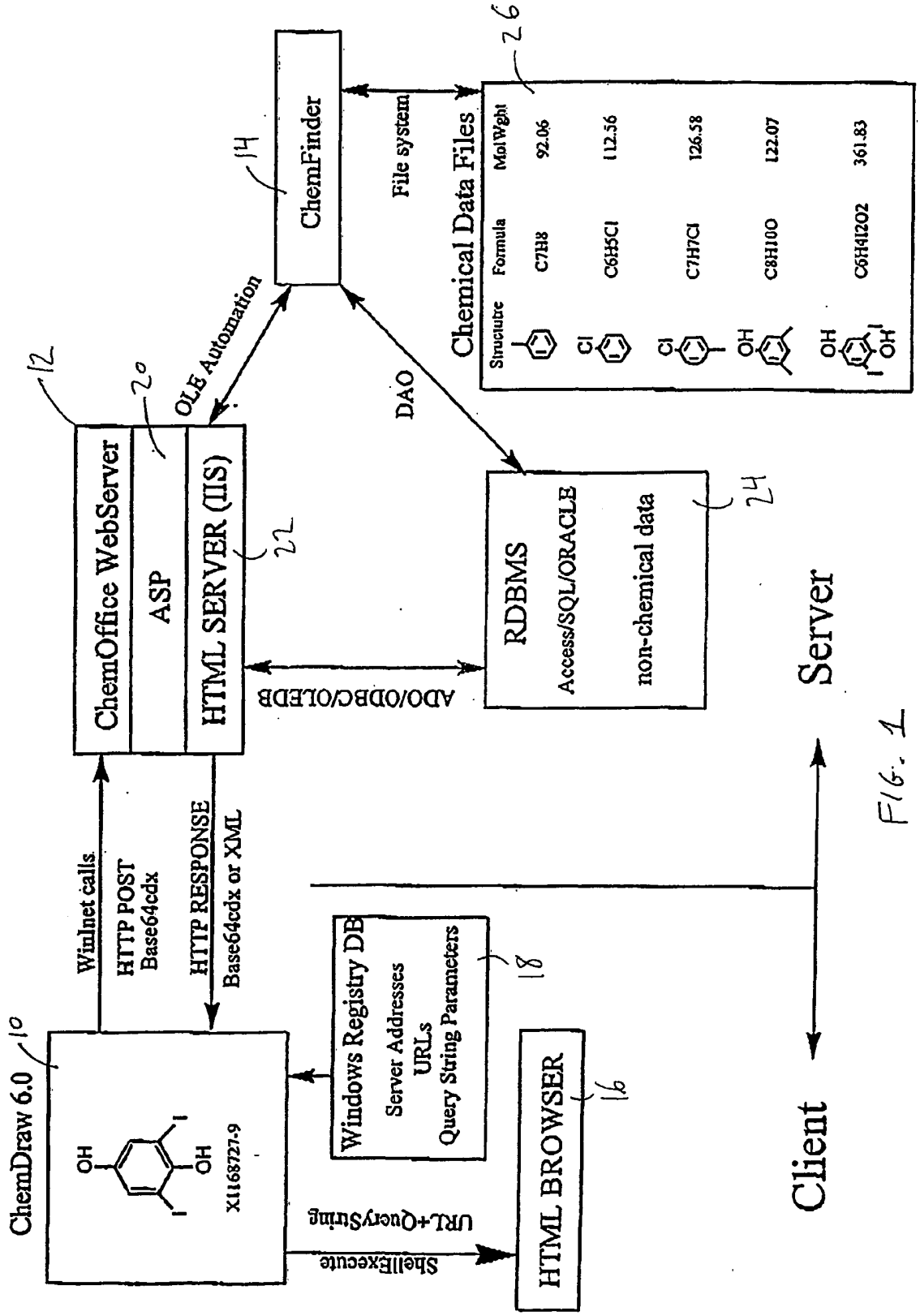

ChemDraw 6.0
10
OH
OH
I
I
X1168727-9
Winlnet calls
HTTP POST
Base64cdx
HTTP RESPONSE
Base64cdx or XML
ChemOffice WebServer
ASP
HTML SERVER (IIS)
12
20
22
OLE Automation
ChemFinder
14
DAO
File system
Chemical Data Files
26
Structure
Formula
MolWght
C7H8
92.06
C6H5Cl
112.56
C7H7Cl
126.58
C8H10O
122.07
C6H4I2O2
361.83
RDBMS
Access/SQL/ORACLE
non-chemical data
24
ADO/ODBC/OLEDB
Windows Registry DB
Server Addresses
URLs
Query String Parameters
18
ShellExecute
URL+QueryString
HTML BROWSER
16
Client
Server

FIG. 1

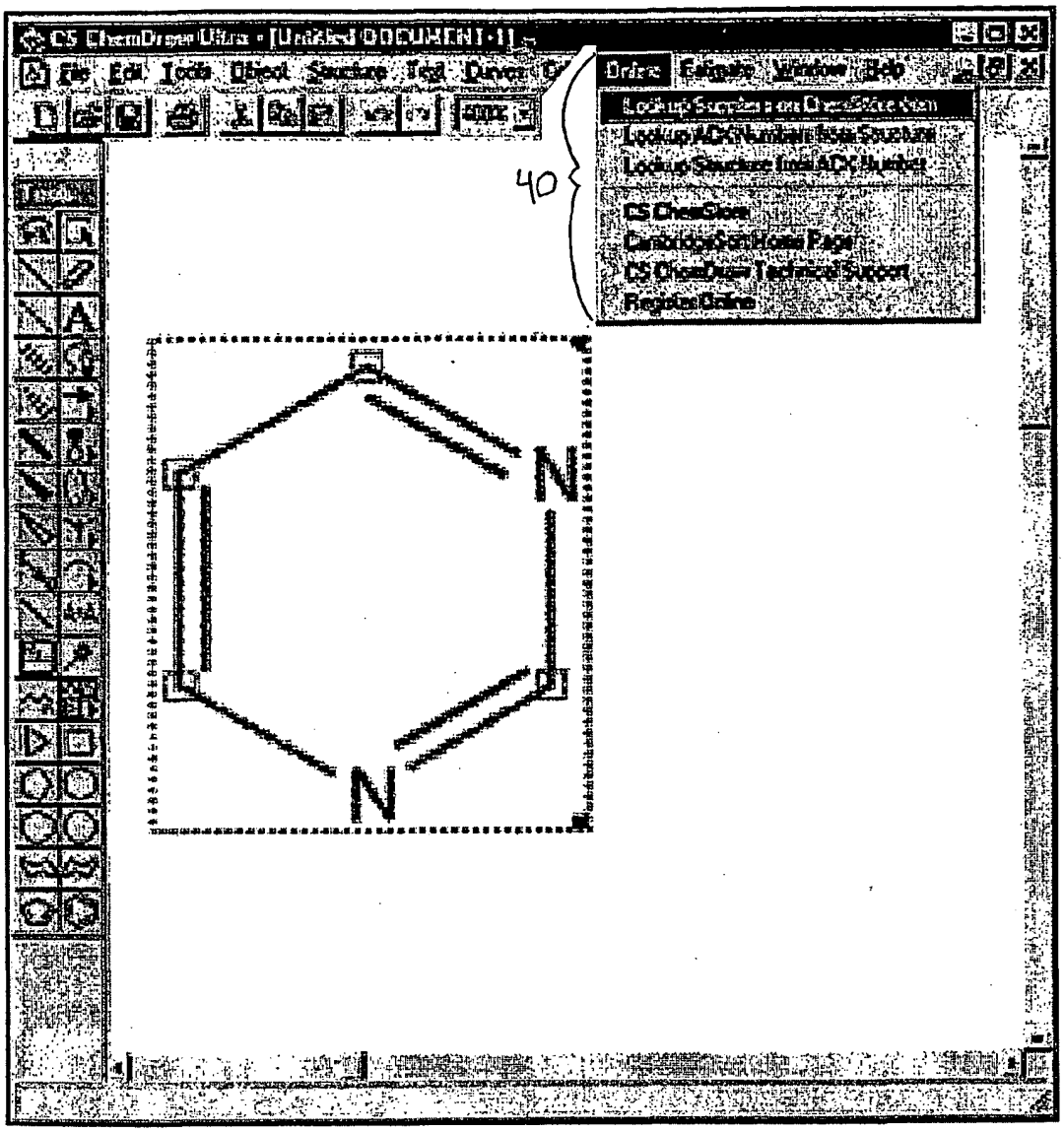


FIG. 2

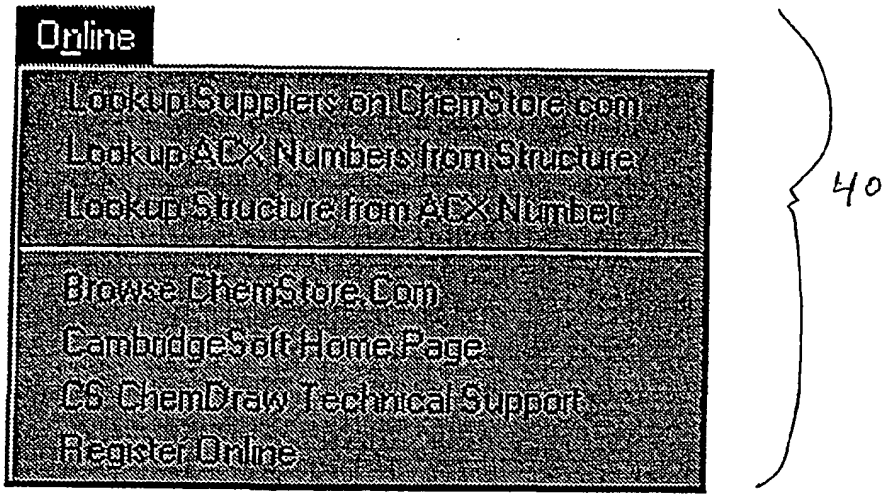

Online
Lookup Suppliers on ChemStore.com
Lookup ACX Numbers from Structure
Lookup Structure from ACX Number
Browse ChemStore.Com
CambridgeSoft Home Page
CS ChemDraw Technical Support
Register Online
40

FIG. 3

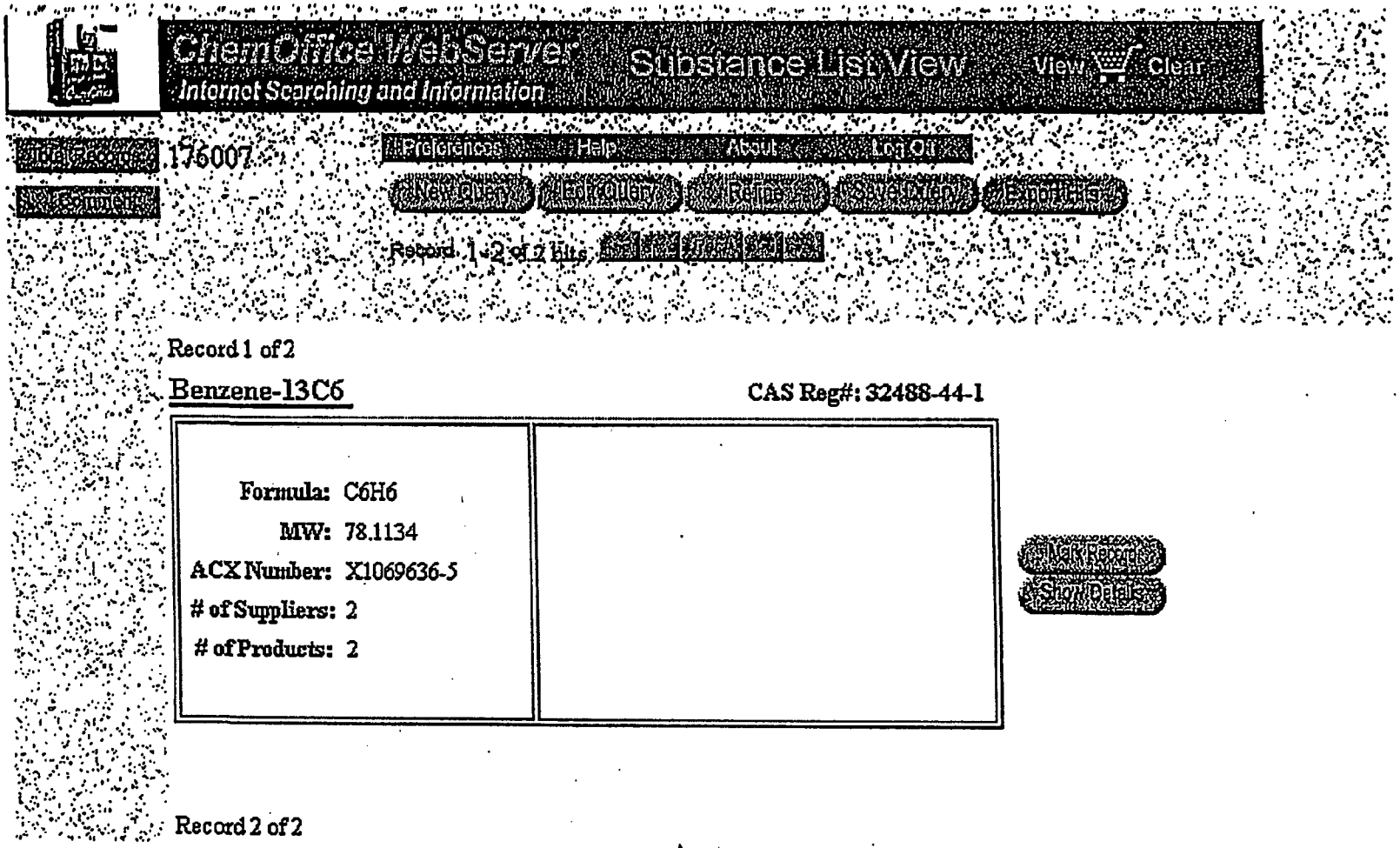

ChemOffice WebServer
Internet Searching and Information
Substance List View
View
Clear
176007
Preferences
Help
About
Log Off
New Query
Edit Query
Refine
Save Query
Export Hits
Record 1-2 of 2 hits
Record 1 of 2
Benzene-13C6
CAS Reg#: 32488-44-1
Formula: C6H6
MW: 78.1134
ACX Number: X1069636-5
# of Suppliers: 2
# of Products: 2
Mark Record
Show Details
Record 2 of 2

FIG. 4

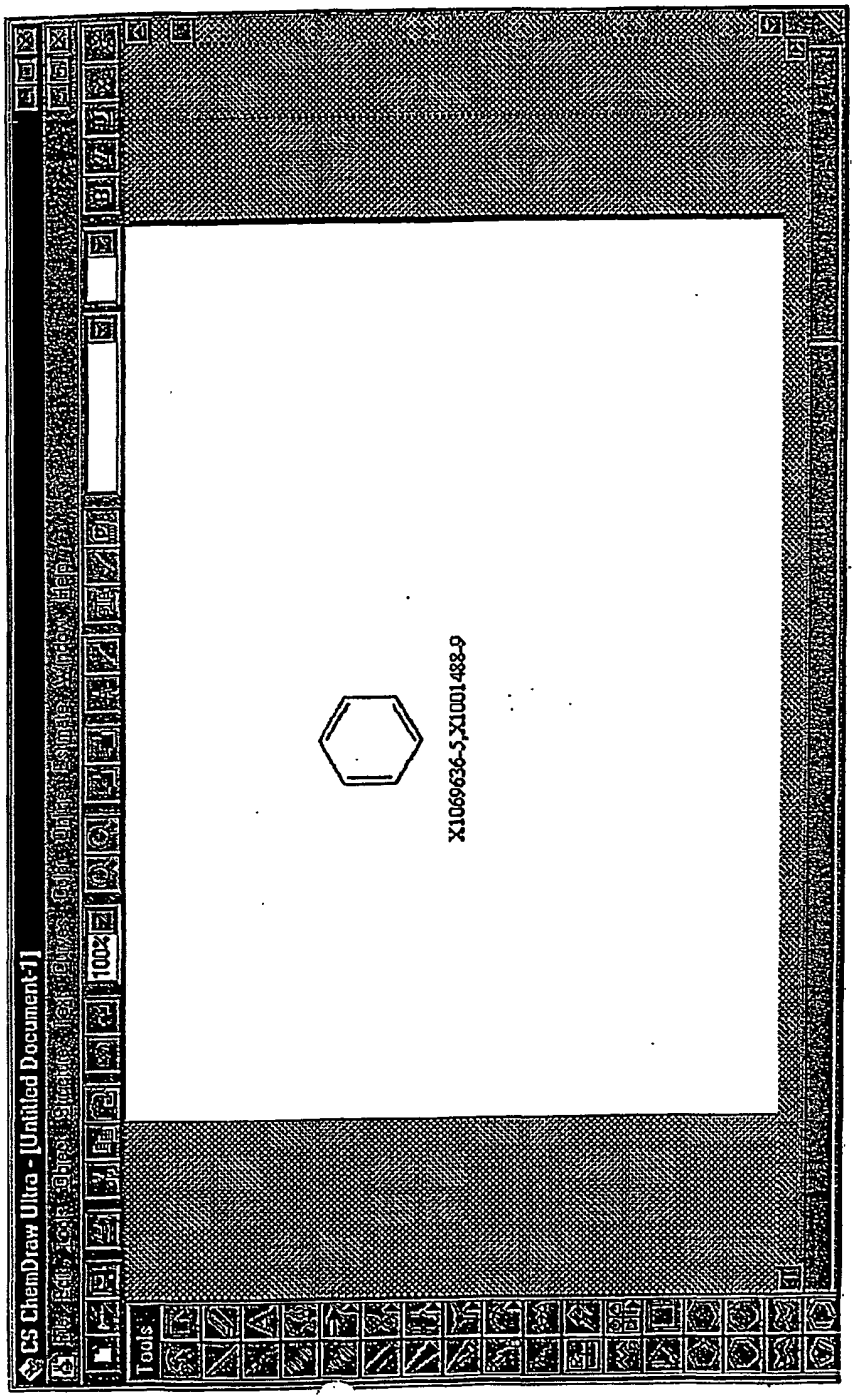

CS ChemDraw Ultra - [Untitled Document-1]
Tools
X1069636-5,X1001488-9

FIG. 5

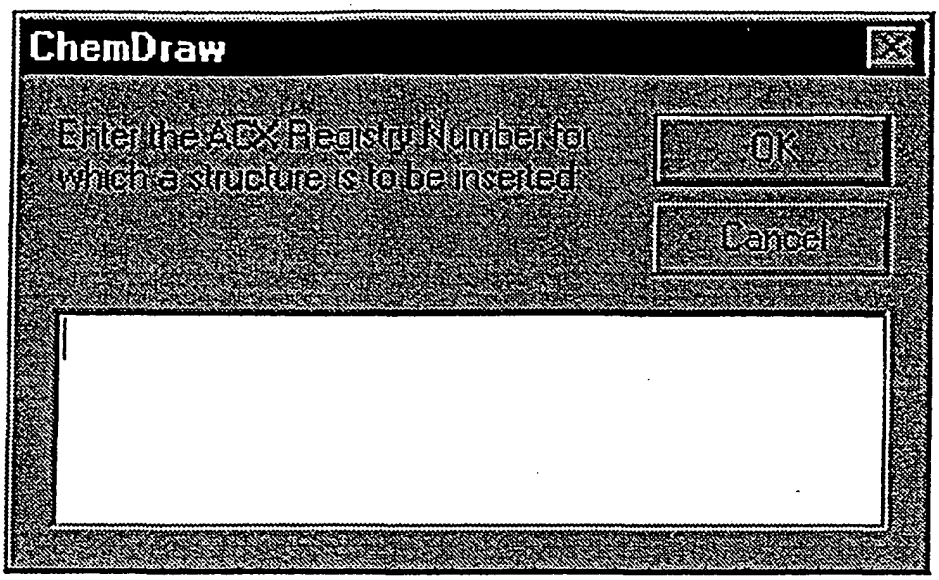

ChemDraw
Enter the ACX Registry Number for which a structure is to be inserted
OK
Cancel

FIG. 6

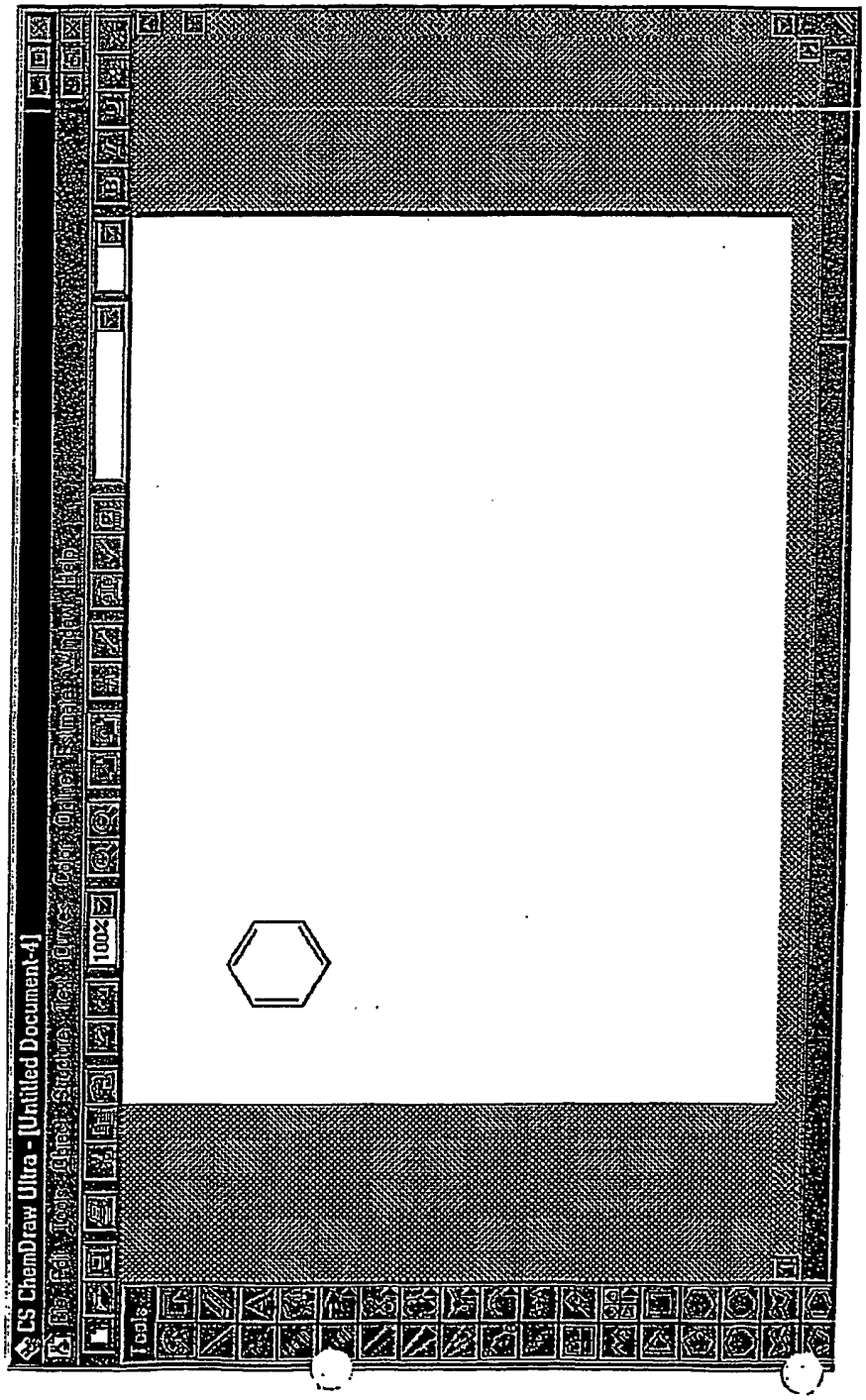
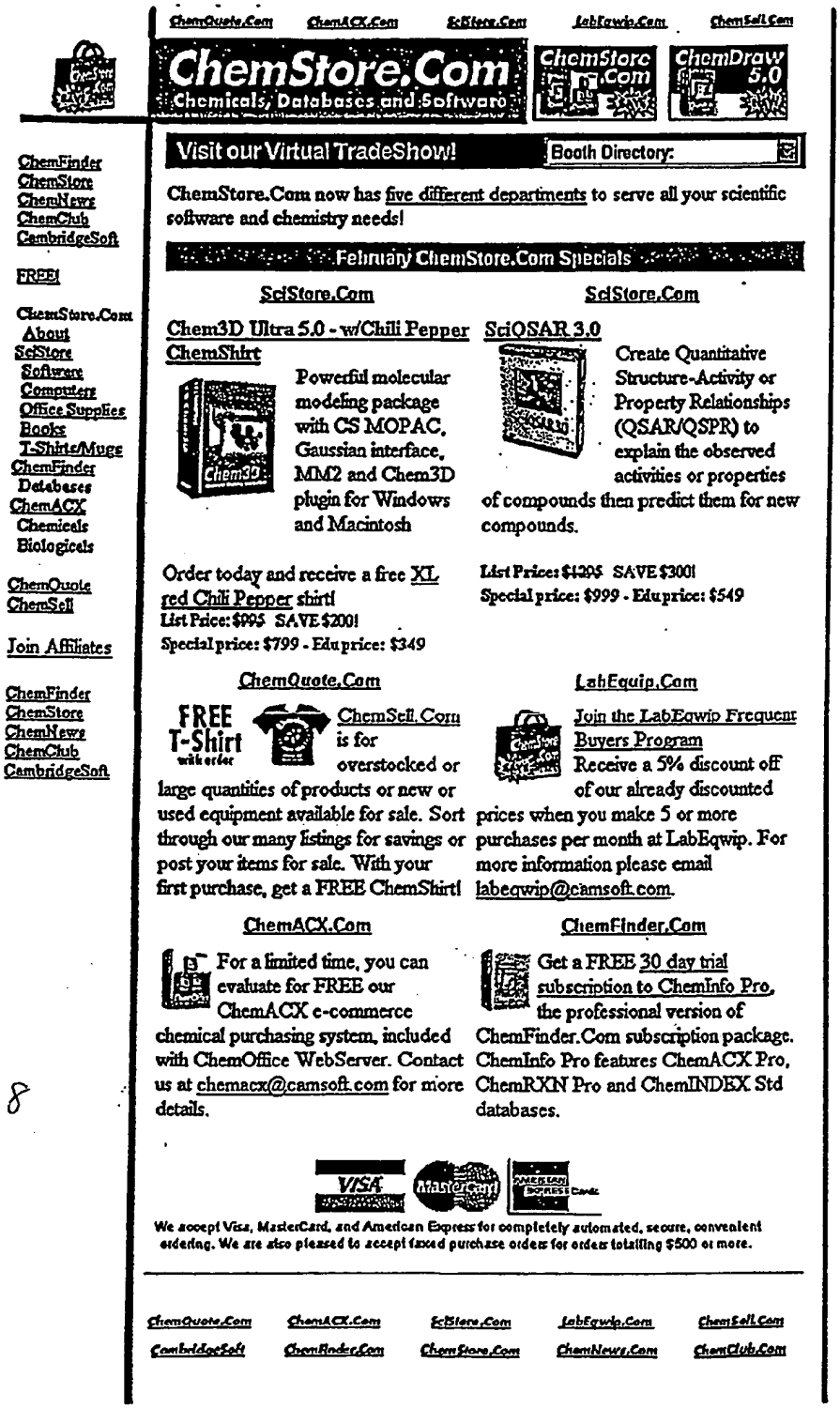


FIG. 7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ChemDraw 5.0
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Databases
ChemACX
Chemicals
Biologicals
ChemQuote
ChemSell
Join Affiliates
ChemFinder
ChemStore
ChemNews
ChemClub
CambridgeSoft
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FIG. 8

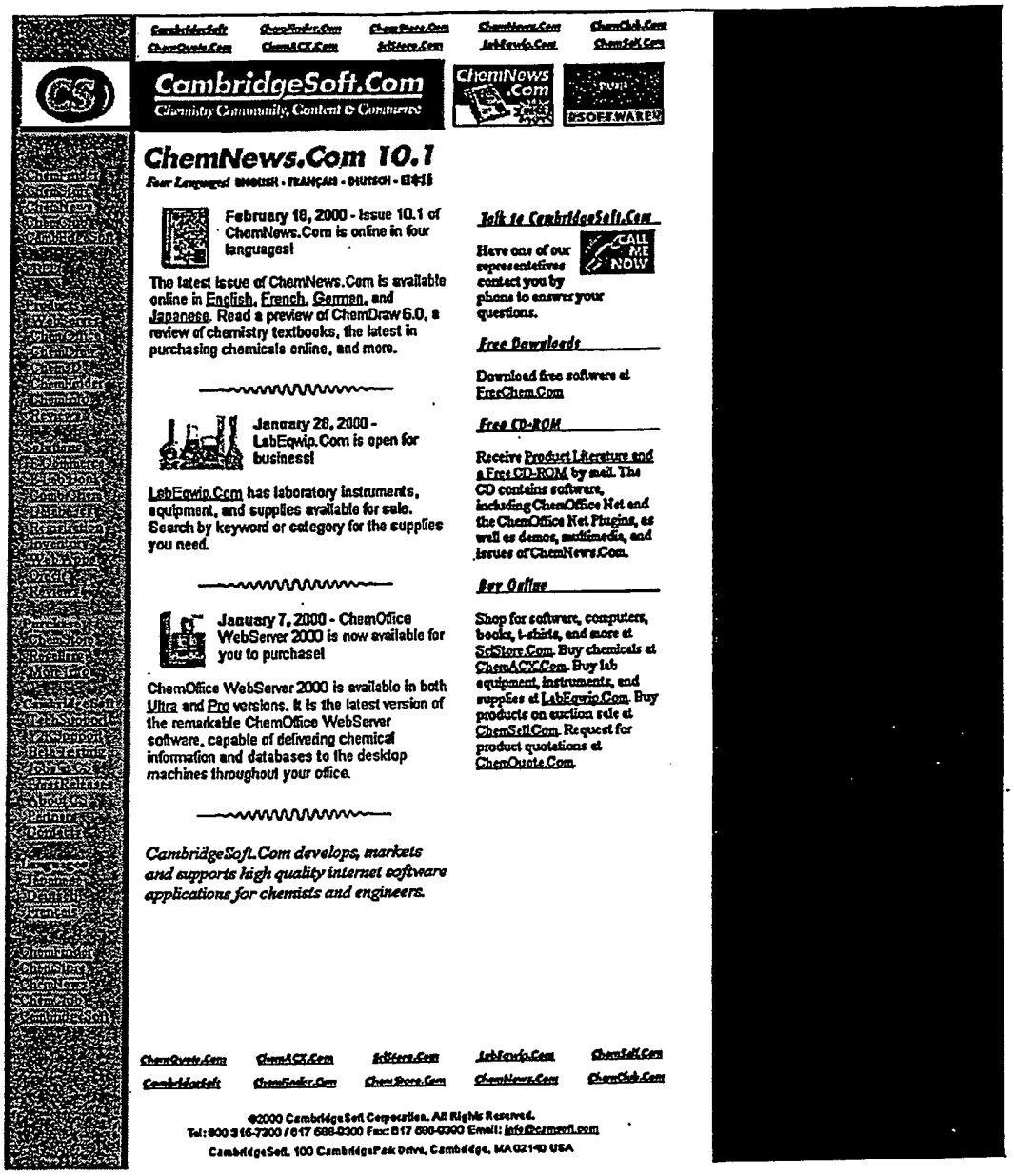

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FIG. 9

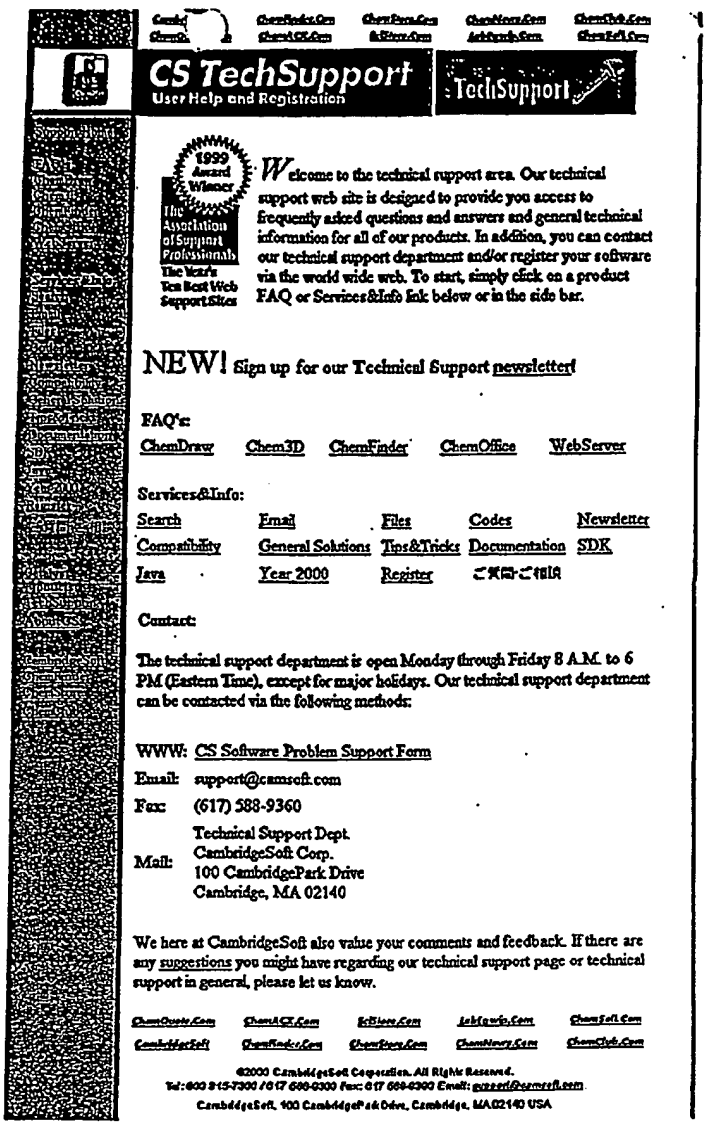

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FIG. 10

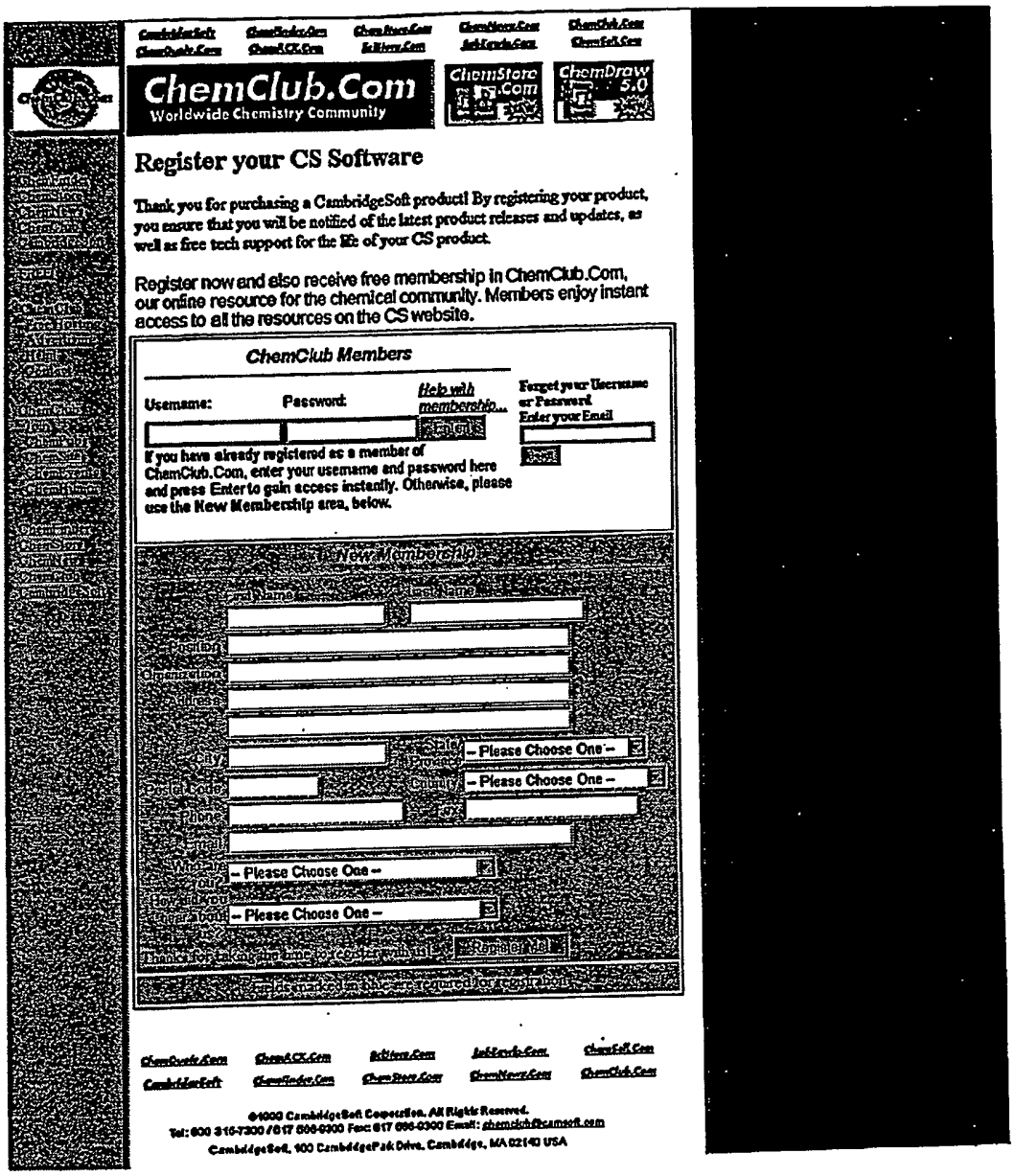
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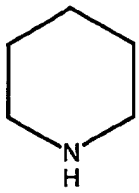
FIG. 11

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01983589  00 00 43 68 65 6D 44 72 61 77 20 36 2E 30 2E 33  ..ChemDraw 6.0.3
01983599  62 39 08 00 15 00 00 00 55 6E 74 69 74 6C 65 64  b9......Untitled
019835A9  20 44 6F 63 75 6D 65 6E 74 2D 31 00 03 32 00 08   Document-1..2..
019835B9  00 FF FF FF FF FF FF 00 00 00 00 00 00 FF FF 00  .ÿÿÿÿÿÿ......ÿÿ.
019835C9  00 00 00 FF FF FF FF 00 00 00 00 00 FF FF 00 00  ...ÿÿÿÿ.....ÿÿ..
019835D9  00 FF FF FF FF 00 00 00 00 FF FF FF FF 00 00 FF  .ÿÿÿÿ....ÿÿÿÿ..ÿ
019835E9  FF 00 09 00 00 01 09 08 00 00 00 68 00 00 00 96  ÿ..........h...-
019835F9  00 02 09 08 00 00 00 4D 02 00 00 3B 03 02 08 10  .......M...;....
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01983629  08 04 00 00 00 1E 00 06 08 04 00 00 00 04 00 07  ................
01983639  08 04 00 00 00 01 00 08 08 04 00 00 00 02 00 09  ................
01983649  08 04 00 33 B3 02 00 0A 08 08 00 03 00 60 00 C8  ...3³........`.È
01983659  00 03 00 0B 08 08 00 04 00 00 00 F0 00 03 00 0D  ...........ð....
01983669  08 00 00 00 08 78 00 00 03 00 00 02 58 02 58 00  .....x......X.X.
01983679  00 00 00 19 0D 13 57 FF A9 FF B2 19 71 13 9E 03  ......W ÿ©ÿ².q.ž.
01983689  67 05 28 03 FC 00 02 00 00 02 58 02 58 00 00 00  g.(.ü.....X.X...
01983699  00 19 0D 13 57 00 01 00 64 00 64 00 00 00 01 00  ....W...d.d.....
019836A9  01 01 01 00 00 00 01 27 0F 00 01 00 01 00 00 00  .......'........
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019836E9  02 10 00 00 00 5E 00 00 00 BD 00 00 00 AE 00 00  .....^...½...®..
019836F9  00 FA 00 00 01 24 00 00 00 02 00 03 00 E4 04 05  .ú...$.......ä..
01983709  00 41 72 69 61 6C 04 00 E4 04 0F 00 54 69 6D 65  .Arial..ä...Time
01983719  73 20 4E 65 77 20 52 6F 6D 61 6E 01 80 0E 00 00  s New Roman.€...
01983729  00 04 02 10 00 00 00 5E 00 00 00 BD 00 00 00 AE  .......^...½...®
01983739  00 00 00 FA 00 0F 08 02 00 01 00 10 08 02 00 01  ...ú............
01983749  00 16 08 04 00 00 00 24 00 18 08 04 00 00 00 24  .......$.......$
01983759  00 19 08 00 00 03 80 0F 00 00 00 00 04 02 10 00  ......€.........
01983769  00 60 00 00 00 BF 00 00 00 AC 00 00 00 F8 00 04  .`...¿...¬...ø..
01983779  80 01 00 00 00 0A 00 02 00 01 00 00 02 08 00 00  €...............
01983789  00 71 00 EC 04 C1 00 37 04 01 00 01 00 00 04 80  .q.ì.Á.7.......€
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019837A9  8F 00 EC 04 C1 00 37 04 01 00 01 00 00 04 80 03  ..ì.Á.7.......€.
019837B9  00 00 00 0A 00 02 00 03 00 00 02 08 00 00 00 9E  ...............ž
019837C9  00 00 00 DB 00 06 80 0D 00 00 00 0A 00 02 00 0D  ...Û..€.........
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019837F9  00 05 00 02 08 00 66 E6 A1 00 00 30 D8 00 04 02  ......fæ¡..0Ø...
01983809  10 00 00 00 9B 00 00 00 D9 00 00 00 AC 00 00 00  ....›...Ù...¬...
01983819  DE 00 00 00 37 04 01 00 01 02 04 02 00 07 00 2B  Þ...7..........+
01983829  04 02 00 01 00 00 00 04 80 04 00 00 00 0A 00 02  ........€.......
```

FIG. 12A

```
01983839  00 04 00 00 02 08 00 00 00 8F 00 13 FB F4 00 37  ............ûô.7
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01983859  05 00 00 02 08 00 00 00 71 00 13 FB F4 00 37 04  ........q..ûô.7.
01983869  01 00 01 00 00 04 80 06 00 00 00 0A 00 02 00 06  ......€.........
01983879  00 00 02 08 00 00 00 62 00 00 00 DB 00 37 04 01  .......b...Û.7..
01983889  00 01 00 00 05 80 07 00 00 00 0A 00 02 00 07 00  .....€..........
01983899  04 06 04 00 01 00 00 00 05 06 04 00 02 00 00 00  ................
019838A9  0A 06 01 00 01 00 00 05 80 08 00 00 00 0A 00 02  ........€.......
019838B9  00 08 00 04 06 04 00 02 00 00 00 05 06 04 00 03  ................
019838C9  00 00 00 0A 06 01 00 01 00 00 05 80 09 00 00 00  ............€ ...
019838D9  0A 00 02 00 09 00 04 06 04 00 03 00 00 00 05 06  ................
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01983939  01 00 00 05 80 0C 00 00 00 0A 00 02 00 0C 00 04  ....€...........
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```

FIG. 12B

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AhAAAABeAAAAvQAAAK4AAAD6AAABJAAAAAIAAwDkBAUAQXJpYWwEAOQEDwBUaW1l
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AAAHDgABAAAAAwBgAMgAAwBOSAQHBgACAAIAAwAFBwEABQACCABm5qEAADDYAAQC
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AAQAAAIIAAAAjwAT+/QANwQBAAEAAASABQAAAAoAAgAFAAACCAAAAHEAE/v0ADcE
AQABAAAEgAYAAAAKAAIABgAAAggAAABiAAAA2wA3BAEAAQAABYAHAAAACgACAAcA
BAYEAAEAAAAFBgQAAgAAAAoGAQABAAAFgAgAAAAKAAIACAAEBgQAAgAAAAUGBAAD
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AAAACgACAAoABAYEAAQAAAAFBgQABQAAAAoGAQABAAAFgAsAAAAKAAIACwAEBgQA
BQAAAAUGBAAGAAAACgYBAAEAAAWADAAAAAoAAgAMAAQGBAAGAAAABQYEAAEAAAAK
BgEAAQAAAAAAAAA

FIG. 13

```
POST HTTP/1.1
/chemacx/chemacx/chemacx_action.asp?dbname=chemacx&dataaction=search_no_gui
Accept: */*
Host: chemdraw.chemacx.com
Referer: Online
User-Agent: CS ChemDraw Ultra 6.0
Cookie: ASPSESSIONIDGGGGGRTD=BELBBHJCLDCFHMOPNDDKFLBO
Content-Length: 1481
Content-Type: application/x-www-form-urlencoded
Cache-Control: no-cache

return_fields=Substance.ACX_ID&struc_search_type=exact&Substance.Structure=
VmpDRDAxMDAEAwIBAAAAAAAAAAAAAAAAAAAAAAMAEgAAAENoZW1EcmF3IDYuMC4z
YjkIABUAAABVbnRpdGxlZCBEb2N1bWVudC0xAAMyAAgA////////AAAAAAAA//8A
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AAAHDgABAAAAAwBgAMgAAwBOSAQHBgACAAIAAwAFBwEABQACCABm5qEAADDYAAQC
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AQABAAAEgAYAAAAKAAIABgAAAggAAABiAAAA2wA3BAEAAQAABYAHAAAACgACAAcA
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AAAACgYBAAEAAAWACQAAAAoAAgAJAAQGBAADAAAABQYEAAQAAAAKBgEAAQAABYAK
AAAACgACAAoABAYEAAQAAAAFBgQABQAAAAoGAQABAAAFgAsAAAAKAAIACwAEBgQA
BQAAAAUGBAAGAAAACgYBAAEAAAWADAAAAAoAAgAMAAQGBAAGAAAABQYEAAEAAAAK
BgEAAQAAAAAAAAA
```

FIG. 14

```
HTTP/1.1 200 OK
Server: Microsoft-IIS/4.0
Date: Wed, 28 Feb 2001 17:34:38 GMT
Content-Type: text/html
Cache-control: private
Transfer-Encoding: chunked

X1001495-4
```

FIG. 15

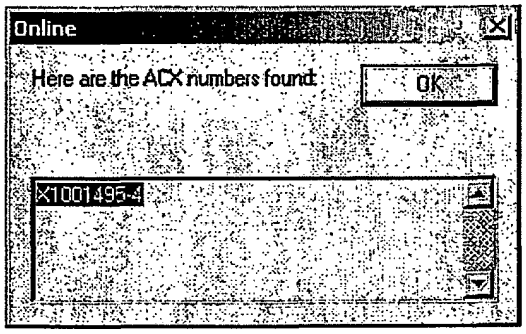

FIG. 16

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
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(43) International Publication Date
7 September 2001 (07.09.2001)

PCT

(10) International Publication Number
WO 01/065415 A3

(51) International Patent Classification[7]: G06F 17/30

(21) International Application Number: PCT/US01/06443

(22) International Filing Date: 28 February 2001 (28.02.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/186,156 29 February 2000 (29.02.2000) US

(71) Applicant: CAMBRIDGESOFT CORPORATION [US/US]; 100 Cambridge Park Drive, Cambridge, MA 02140 (US).

(72) Inventor: RUBENSTEIN, Stewart, D.; 21 Beacon Heights Drive, Newton Center, MA 02159 (US).

(74) Agents: REYES, Jason, A. et al.; Hale and Dorr LLP, 60 State Street, Boston, MA 02109 (US).

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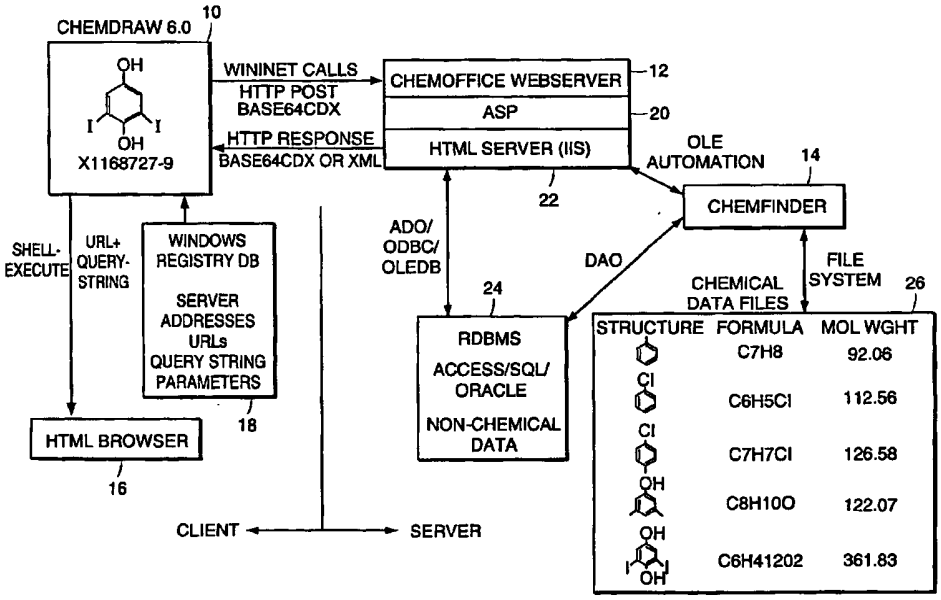
(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
— *with international search report*
— *before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments*

(88) Date of publication of the international search report:
29 August 2002

[Continued on next page]

(54) Title: MANAGING CHEMICAL INFORMATION AND COMMERCE



(57) Abstract: A description of a chemical substance is acquired and a user's selection of a user interface menu item is detected. The user interface menu item pertains to a Web server having access to data for chemical substances. Based on the detection, a request is submitted to the Web server for information based on the description of the chemical substance. A response is received from the Web server that includes data pertaining to the chemical substance. Ouput data is derived from the data pertaining to the chemical substance.

WO 01/065415 A3

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INTERNATIONAL SEARCH REPORT

Internati Application No
PCT/US 01/06443

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 G06F17/30

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
EPO-Internal, WPI Data, PAJ, INSPEC, COMPENDEX, IBM-TDB

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	IHLENFELDT W-D ET AL: "BEYOND THE HYPERACTIVE MOLECULE: SEARCH, SALVAGE AND VISUALIZATION OF CHEMICAL INFORMATION FROM THE INTERNET" PACIFIC SYMPOSIUM ON BIOCOMPUTING '96. HAWAII, JAN. 3 - 6, 1996, SINGAPORE, WORLD SCIENTIFIC, SI, vol. SYMP. 1, 3 January 1996 (1996-01-03), pages 384-395, XP000751937 ISBN: 981-02-2578-4 section 4: Application Examples figures 1-5 --- -/--	1-14

[X] Further documents are listed in the continuation of box C.

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Date of the actual completion of the international search	Date of mailing of the international search report
27 June 2002	04/07/2002

Name and mailing address of the ISA	Authorized officer
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X	ERTL P ET AL: "WWW-BASED CHEMICAL INFORMATION SYSTEM" JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM), ELSEVIER SCIENCE PUBLISHERS B.V., AMSTERDAM, NL, vol. 419, 8 December 1997 (1997-12-08), pages 113-120, XP000957419 ISSN: 0166-1280 Section 1: Introduction figures 1-7 ---	1-14
A	US 5 978 804 A (DIETZMAN GREGG R) 2 November 1999 (1999-11-02) column 2, line 64 -column 3, line 67 ---	1,13,14
A	US 6 023 659 A (AKERBLOM INGRID E ET AL) 8 February 2000 (2000-02-08) column 2, line 16 -column 4, line 20 -----	1,13,14

INTERNATIONAL SEARCH REPORT

Information on patent family members

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PCT/US 01/06443

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
US 5978804 A	02-11-1999	NONE	
US 6023659 A	08-02-2000	US 6363399 B1	26-03-2002
		US 5953727 A	14-09-1999
		US 6189013 B1	13-02-2001

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

CORRECTED VERSION

(19) World Intellectual Property Organization
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(43) International Publication Date
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(72) Inventor: RUBENSTEIN, Stewart, D.; 21 Beacon Heights Drive, Newton Center, MA 02159 (US).

(74) Agents: REYES, Jason, A. et al.; Hale and Dorr LLP, 60 State Street, Boston, MA 02109 (US).

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(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
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(88) Date of publication of the international search report:
29 August 2002

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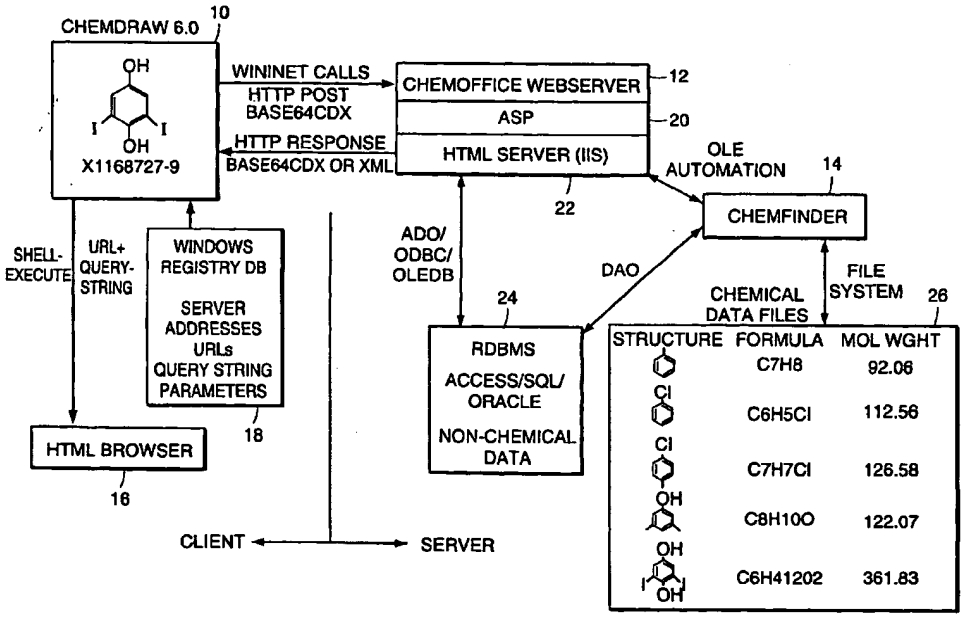
(54) Title: MANAGING CHEMICAL INFORMATION AND COMMERCE



(57) Abstract: A description of a chemical substance is acquired and a user's selection of a user interface menu item is detected. The user interface menu item pertains to a Web server having access to data for chemical substances. Based on the detection, a request is submitted to the Web server for information based on the description of the chemical substance. A response is received from the Web server that includes data pertaining to the chemical substance. Ouput data is derived from the data pertaining to the chemical substance.

WO 01/065415 A3

(48) Date of publication of this corrected version:
3 January 2003

(15) Information about Correction:
see PCT Gazette No. 01/2003 of 3 January 2003, Section II

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

MANAGING CHEMICAL INFORMATION AND COMMERCE

This application claims the benefit of United States Provisional Application Serial No. 60/186,156 entitled "MANAGING CHEMICAL PRODUCT COMMERCE", filed on February 29, 2000, which is incorporated herein by reference.

Background of the Invention

This application relates to managing chemical information and commerce.

A chemistry oriented application program such as a chemical drawing program allows chemical information to be handled as computer data by a computer. A chemical drawing program typically allows a user to cause chemical structural information and chemical reaction information to be displayed on a computer screen and printed out on a computer printer. If a user has chemical information in the application program that is relevant to another application program, the user typically can use the cut and paste capabilities of the application program to copy the relevant information to the other application program. If one of the application programs is a Web browser interacting with a Web server, the user typically can use the cut and paste capabilities to share information between the Web browser and the other application program, and can thereby, in a limited way, share information between the Web server and the other application program. However, existing chemically oriented application programs provide inadequate abilities to access chemical information that is stored in different formats or in remote locations.

Summary of the Invention

Methods and systems are provided for managing chemical information and commerce. In particular, an external query capability allows a chemistry oriented application program to query an external entity such as a chemical information external database using

the Hypertext Transfer Protocol ("HTTP"), to produce information management and commerce management results not otherwise realizable by the application program.

Different aspects of the invention allow one or more of the following. An application program having chemical information can submit that information in a query to a remote chemical database and receive and incorporate a response from the database, without requiring the user to run or exercise another application program such as a Web browser. A user can provide chemical information in one form (e.g., structural) to an application program which can submit the information to another entity such as a remote database in a different form (e.g., textual) that is meaningful to the other entity, and that can lead to retrieval of information that is useful to the user. The capabilities of a chemistry oriented software tool can be linked to, and thereby applied to, a remote organized set of chemical information to produce analytical and commercial results such as reports and purchasing lists based on the remote organized set of chemical information.

Other features and advantages will become apparent from the following description, including the drawings, and from the claims.

Brief Description of the Drawings

Fig. 1 is a block diagram of a computer-based system.

Figs. 2-11, 16 are illustrations of output displays that may be produced by the computer based system.

Figs. 12A-15 are illustrations of data forms that may be used in the computer based system.

Detailed Description

A chemistry oriented application program has an external query capability that allows the program to query an external entity such as a chemical information external database.

Fig. 1 illustrates an example system in which a chemical drawing application program 10 (in this example, ChemDraw 6.0, provided by CambridgeSoft Corporation of Cambridge, Massachusetts) serves as the application program and uses the external query capability to acquire information via HTTP from a Web server 12 (in this example, ChemOffice WebServer, provided by CambridgeSoft Corporation of Cambridge, Massachusetts) linked to a chemical information database 14 (in this example, ChemFinder, provided by CambridgeSoft Corporation of Cambridge, Massachusetts). Although these particular chemistry oriented programs are provided to illustrate the present invention, other applications programs, Web servers, databases, and other programs may be used as well or instead.

In the example system, which is a Microsoft Windows implementation using ChemDraw, ChemDraw can, if necessary, invoke a Web browser 16 (e.g., see the third and fourth examples below) and can retrieve information including server addresses, uniform resource locators (URLs), and query string parameters from a Windows registry database ("Windows registry") 18. ChemDraw can use WinInet calls to post HTTP requests to the ChemOffice Webserver, and receives responses in HTTP form. WinInet, which is supplied as part of the Windows operating system, is a set of functions (also known as calls, procedures, and subroutines) in an Internet application programming interface (API) that may be implemented as dynamic link library file (DLL). A DLL provides a library of functions that applications link to and call as regular function calls.

The ChemOffice WebServer uses Active Server Pages ("ASP") software 20 and Hypertext Markup Language (HTML) server software known as Internet Information Server ("IIS") 22 to interact with ChemFinder via Object Linking and Embedding (OLE) Automation, and with a relational database management system ("RDBMS") 24. (Other interaction mechanisms may be used in place of or in addition to OLE Automation.) Web pages managed by ChemOffice WebServer may be formatted according to HTML or XML (Extensible Markup Language). Additionally, Web pages may be formatted as, for example, active server page text files ("ASP files") compatible with the ASP software. An ASP file may rely on a combination of HTML or XML and a scripting language such as VBScript or JavaScript.

The interaction with the RDBMS is implemented using one or more data access technologies such as Open Database Connectivity (ODBC), Active Data Objects (ADO), and OLEDB. ODBC is a standard for accessing different database systems from a high level programming language application, and enables applications to submit statements to ODBC using structured query language (SQL), which statements are then translated to the particular SQL commands that are used by the specific underlying database product.

The RDBMS includes non-chemical data such as substance prices. ChemFinder is able to retrieve chemical information such as chemical structure data ("chemical structure"), chemical formulas, and molecular weights from chemical data files 26, and interacts with the RDBMS using, e.g., ADO technology. According to ADO, data from a database is mapped into active data objects which perform the actual queries to the database. This approach provides substantial abstraction by limiting exposure only to the resultant objects.

ChemDraw communicates with an external chemical database server as now described with reference to multiple examples including an example illustrating how ChemDraw may be used to purchase chemicals online at the Available Chemicals Xchange web site (ChemACX.com). ChemDraw can initiate a database query based on either a chemical structure drawing or a simple text string. (Other application programs may use other data formats.) The response provided by the chemical database server can be a simple text response, a chemical structure, or a complex record set containing a combination of chemical and non-chemical data. The process by which ChemDraw handles a query differs slightly depending on the request/response method that is available.

In a first example, a chemical structure drawing is used to retrieve a plain text response. Using ChemDraw, the user creates a drawing of a molecule which is stored as chemical structure by ChemDraw in a native binary format known as cdx.

When the user selects "Look up ACX number from structure" from an online menu 40 (Figs. 2-3), which is a pulldown menu in ChemDraw, ChemDraw converts the chemical structure data from the cdx format to an ASCII text representation. The cdx-to-ASCII conversion is accomplished via a base64 encoding process with a subsequent URL encoding for safe transport over the HTTP protocol. Base64 is an encoding scheme defined by the Multipurpose Internet Mail Extensions (MIME) standard, and is defined to provide robustness to binary data that is expected to confront transformations while traversing the Internet. Base64 encoding converts binary data into alphanumeric characters. For example, binary data such as "110110001011010100000101" may be encoded as textual data "sLUF" which may be transmitted across the Internet.

ChemDraw uses configuration information stored in the Windows registry database to derive a target URL, i.e., a URL pointing to a remote chemical database server. Using the URL derived from the registry information and the URL encoded ASCII text representation of the chemical structure drawn by the user, ChemDraw uses WinInet to post an HTTP request. The converted chemical structure data is passed in the body of the HTTP request.

The remote chemical database server responds with a comma delimited text string containing one or more ACX numbers (e.g., ACX number X1069636-5 shown in Fig. 4) corresponding to the chemical structure drawn by the user. (ACX numbers are product identifiers described in two commonly assigned co-pending applications filed May 5, 2000: 09/565,085 entitled "DERIVING PRODUCT INFORMATION", and 09/565,810 entitled "MANAGING PRODUCT INFORMATION", which applications are incorporated herein by reference.)

ChemDraw captures the server's response by reading the HTTP response.

As shown by example in Fig. 5, the ACX numbers received from the server are displayed by ChemDraw on the ChemDraw canvas in a text box displayed near, e.g., immediately below, the user's chemical structure drawing.

In a second example, a plain text input value is used to retrieve a chemical structure drawing. In particular, a reverse version of the first example above can be accomplished by providing a valid ACX number and retrieving the corresponding chemical structure. In this example, the user selects "Lookup structure from the ACX number" in the ChemDraw 6.0 online menu.

A dialog box shown by example in Fig. 6 opens and prompts the user to enter an ACX number.

ChemDraw retrieves target URL information from the Windows registry and builds an HTTP request. In this case, the payload of the HTTP request is a string containing the ACX number, which is appended to the URL as a query string. The HTTP response returned by the remote server contains a URL encoded base64 text representation of a chemical structure. ChemDraw decodes the text representation and displays the structure on its canvas as a native ChemDraw picture shown by example in Fig. 7.

In a third example, an external HTML browser session is initiated with a remote server. Although ChemDraw is able to access remote servers by directly managing HTTP calls, ChemDraw can also delegate interactions with the server to an external HTML browser. A user selects a "Browse ChemStore.Com" online menu item in ChemDraw, which causes the default HMTL browser to be launched on the user's computer and directed to load a Web page from ChemStore.com as shown by example in Fig. 8.

ChemDraw proceeds in the third example as follows. ChemDraw builds a URL from configurable data stored in the Windows registry. ChemDraw issues a call to ShellExecute with the target URL as a parameter, which causes the user's default browser to open and load the page specified by the URL. (In Microsoft Windows, the ShellExecute function either launches the specified application program, or, if the program is already executing, makes the program the current window.)

Complex URLs corresponding to user specific server pages can be built by incorporating data received from previous queries using techniques described in the first and second examples above. For example, a specific page from a chemical supplier's catalog can be retrieved based on a structure of a molecule drawn by the user.

In a fourth example, a user accomplishes online purchasing of chemicals by starting from ChemDraw. The first and second examples above illustrate how ChemDraw can send or receive a chemical structure or text data to or from a remote chemical database server and display the results directly in ChemDraw's drawing area. When the results of a query are expected to be lengthy or complex, ChemDraw causes a standard HTML browser to handle the display instead.

In this example, chemicals are purchased online from ChemACX.com. As described in the first example above, the user draws a molecule and selects the "Lookup suppliers from ChemACX.com" online menu item.

The chemical structure drawn by the user is used in this example to identify the substance for which purchasing information is to be fetched. Thus, the procedure is as described in the first example above, except that the value returned by the server is a substance identifier that is not meaningful to the end user, and therefore is not displayed, but is used as an intermediate value for querying a Web based catalog.

Specifically, the substance identifier is posted to a remote server to obtain the desired purchasing information. The requested result set is to be displayed in an external browser window. Accordingly, ChemDraw uses techniques described above in the third example to build a URL pointing the specific catalog page at ChemACX.Com which contains information about the desired substance. This URL is built from server target information stored in the Windows registry database and from the unique substance identifier fetched from the server in the initial step described above.

ChemDraw opens the user's default external browser and automatically causes the browser to load the appropriate catalog page. The user can use the browser to navigate the

available purchasing information and initiate the online ordering process from within the browser.

In a specific implementation in which the user is presented with a list of suppliers and prices in a Web browser window, the user can then check off the supplier and desired quantity, which causes a corresponding shopping cart construct to be created, ready for submission for purchase completion.

The online menu may also be configured to retrieve other pieces of data based on a selected structure, such as specific compound identification numbers from specific manufacturers.

Figs. 12A-16 illustrate a specific example of data transformations referenced above, with respect to an example interaction when a user draws a structure and selects the "Find ACX Numbers from Structure" online menu item. Figs. 12A-12B illustrate a chemical structure and its corresponding binary CDX form. Fig. 13 illustrates the base64 encoded form corresponding to Figs. 12A-12B. Fig. 14 illustrates the encoded request corresponding to Fig. 13. Fig. 15 illustrates the response from the server corresponding to Fig. 14. Fig. 16 illustrates a display provided to the user corresponding to Fig. 15.

Figs. 9-11 illustrate examples of other pages that may be retrieved by selection of, respectively, the "CambridgeSoft Home Page", "CS ChemDraw Technical Support", and "Register Online" online menu items shown in Figs. 2-3.

All, or a portion, of the procedures described above may be implemented in hardware or software, or a combination of both. In at least some cases, it is advantageous if the technique is implemented in computer programs executing on one or more programmable computers, such as a personal computer running or able to run an operating system such as

Unix, Linux, Microsoft Windows 95, 98, 2000, or NT, or Macintosh OS, that each include a processor, a storage medium readable by the processor (including volatile and non-volatile memory and/or storage elements), at least one input device such as a keyboard, and at least one output device. Program code is applied to data entered using the input device to perform the technique described above and to generate output information. The output information is applied to one or more output devices such as a display screen of the computer.

In at least some cases, it is advantageous if each program is implemented in a high level procedural or object-oriented programming language such as Perl, C, C++, or Java to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

In at least some cases, it is advantageous if each such computer program is stored on a storage medium or device, such as ROM or optical or magnetic disc, that is readable by a general or special purpose programmable computer for configuring and operating the computer when the storage medium or device is read by the computer to perform the procedures described in this document. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner.

Other embodiments are within the scope of the following claims. For example, a more general range of services may be provided. A query may be performed on local or remote databases, and may be used in the derivation of a non-exact query or a non-structural query. For instance, in the case of ChemDraw which provides property prediction facilities,

such facilities may be used to predict physical characteristics of a molecule of interest, and local or remote databases may be searched for substances having similar properties. The online menu may be used in another application program such as a spreadsheet program. For instance, in the case of the spreadsheet program, the program may store a shopping list of chemical products, and the online menu may include a selectable item for retrieving price information for each listed product from a remote chemical information database and embedding the retrieved price information in the shopping list.

What is claimed is:

1. A method for use in managing chemical information, comprising:

acquiring a description of a chemical substance;

detecting a user's selection of a user interface menu item pertaining to a Web server having access to data for chemical substances;

based on the detection, submitting, to the Web server, a request for information based on the description of the chemical substance;

receiving a response from the Web server, the response including data pertaining to the chemical substance; and

deriving output data from the data pertaining to the chemical substance.

2. The method of claim 1, wherein the description of the chemical substance includes a structural description of the chemical substance.

3. The method of claim 1, wherein the description of the chemical substance includes a textual description of the textual substance.

4. The method of claim 1, wherein the output data includes structural output data.

5. The method of claim 1, wherein the output data includes textual output data.

6. The method of claim 1, wherein the output data includes commercial product data.

7. The method of claim 1, wherein the user interface item is provided by a chemistry oriented application program.

8. The method of claim 7, wherein the chemistry oriented application program includes a chemical drawing program.

9. The method of claim 1, further comprising

formatting at least a portion of the request for information according to the HTTP protocol.

10. The method of claim 1, further comprising

decoding at least a portion of the response from the Web server according to the HTTP protocol.

11. The method of claim 1, further comprising

presenting a user interface window that includes a display corresponding to the description of the chemical substance and another display derived from the output data.

12. The method of claim 1, further comprising

causing a new Web browser window to be displayed; and

causing a display derived from the output data to be displayed in the new Web browser window.

13. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to manage chemical information, the instructions causing the system to:

acquire a description of a chemical substance;

detect a user's selection of a user interface menu item pertaining to a Web server having access to data for chemical substances;

based on the detection, submit, to the Web server, a request for information based on the description of the chemical substance;

receive a response from the Web server, the response including data pertaining to the chemical substance; and

derive output data from the data pertaining to the chemical substance.

14. A system for use in managing chemical information, comprising:

a Web server having access to data for chemical substances; and

a chemistry oriented application program providing a user interface menu item linked to the Web server.

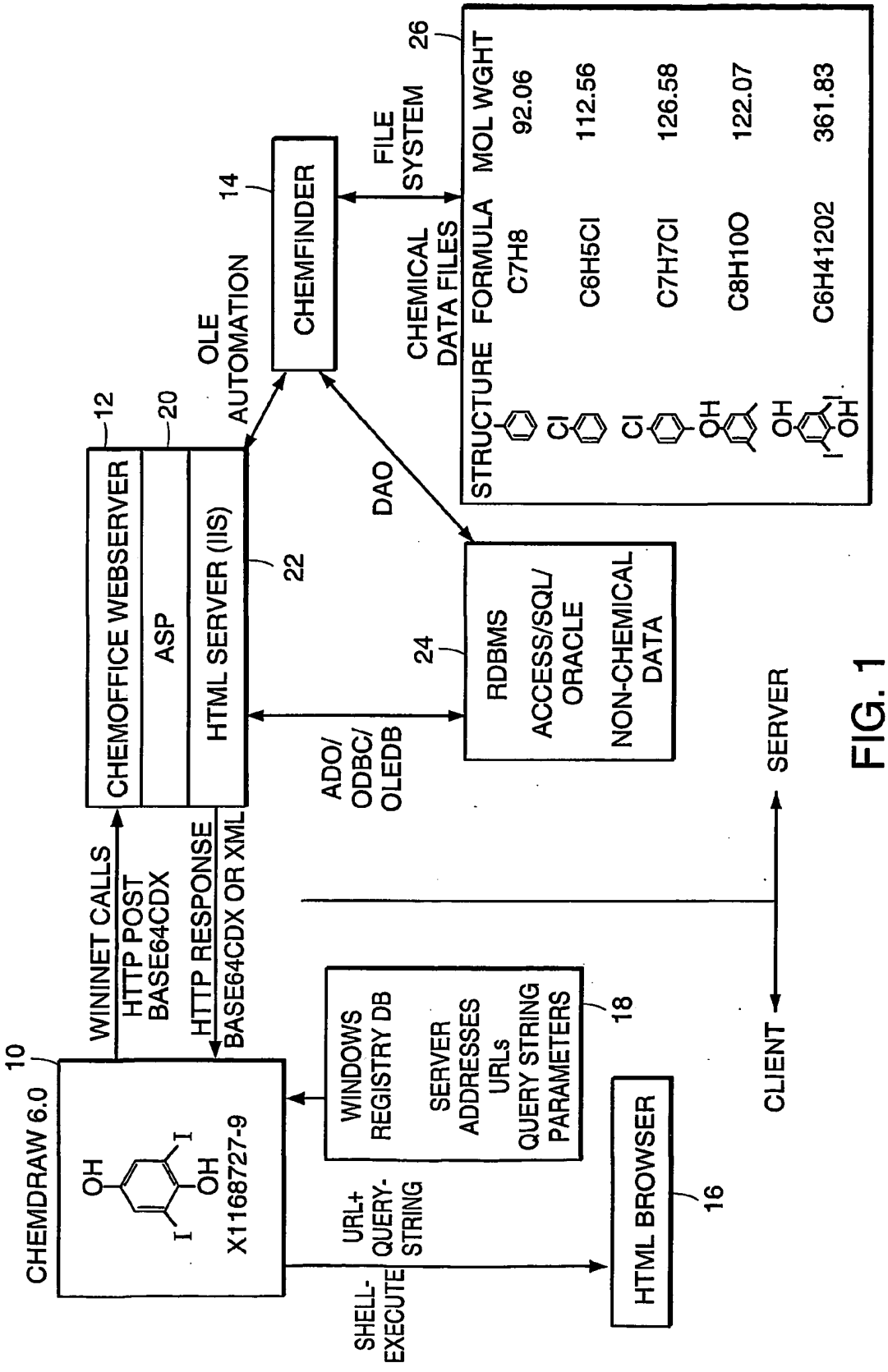

CHEMDRAW 6.0
10
X1168727-9
WININET CALLS
HTTP POST
BASE64CDX
HTTP RESPONSE
BASE64CDX OR XML
CHEMOFFICE WEBSERVER
ASP
HTML SERVER (IIS)
12
20
22
OLE AUTOMATION
14
CHEMFINDER
FILE SYSTEM
26
CHEMICAL DATA FILES
STRUCTURE
FORMULA
MOL WGHT
C7H8
92.06
C6H5Cl
112.56
C7H7Cl
126.58
C8H10O
122.07
C6H41202
361.83
DAO
ADO/ ODBC/ OLEDB
24
RDBMS
ACCESS/SQL/ ORACLE
NON-CHEMICAL DATA
WINDOWS REGISTRY DB
SERVER ADDRESSES
URLs
QUERY STRING PARAMETERS
18
URL+ QUERY-STRING
SHELL-EXECUTE
HTML BROWSER
16
SERVER
CLIENT

FIG. 1

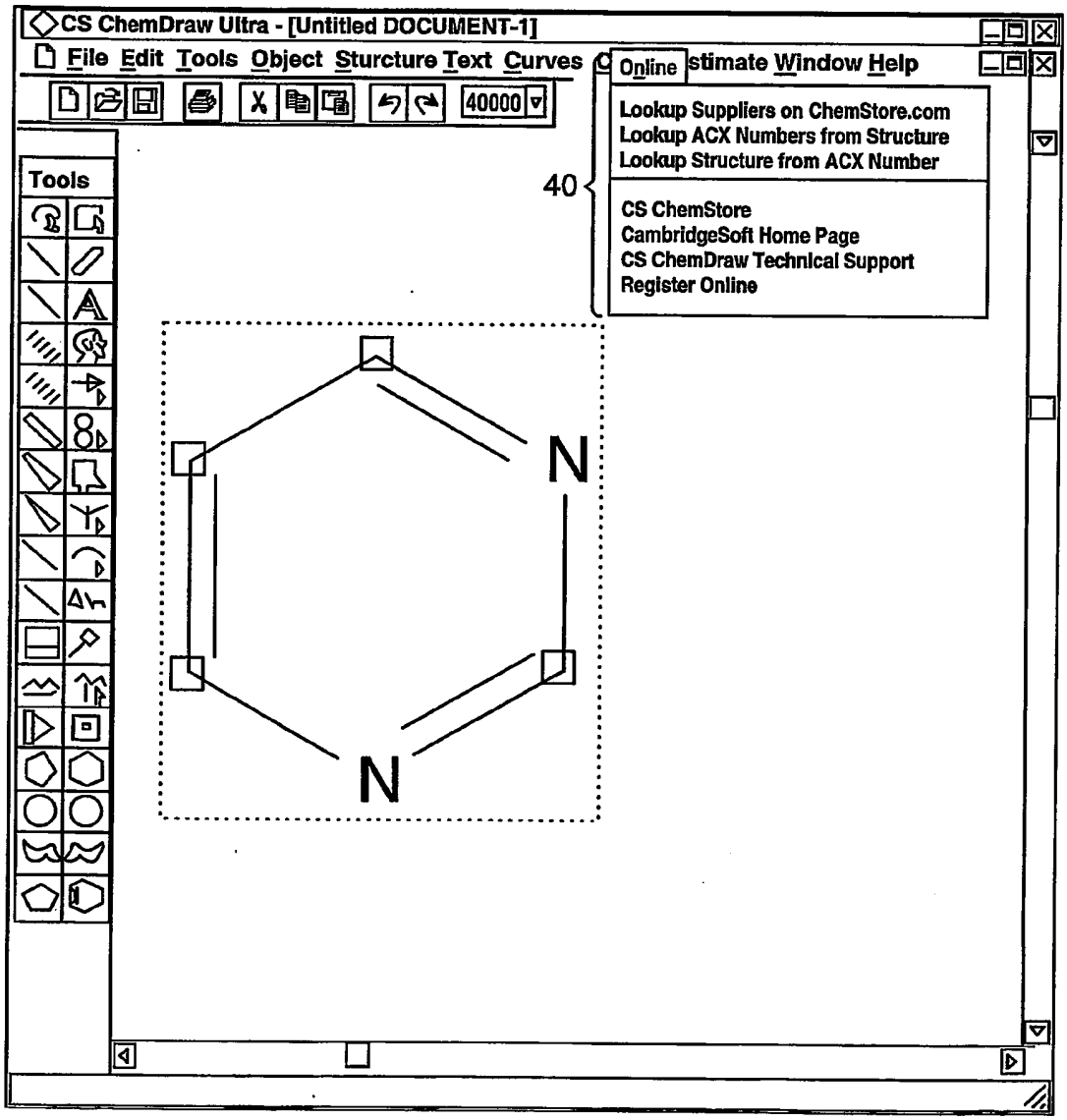

CS ChemDraw Ultra - [Untitled DOCUMENT-1]
File Edit Tools Object Sturcture Text Curves
Online
stimate Window Help
40000
Tools
40
Lookup Suppliers on ChemStore.com
Lookup ACX Numbers from Structure
Lookup Structure from ACX Number
CS ChemStore
CambridgeSoft Home Page
CS ChemDraw Technical Support
Register Online
N
N

FIG. 2

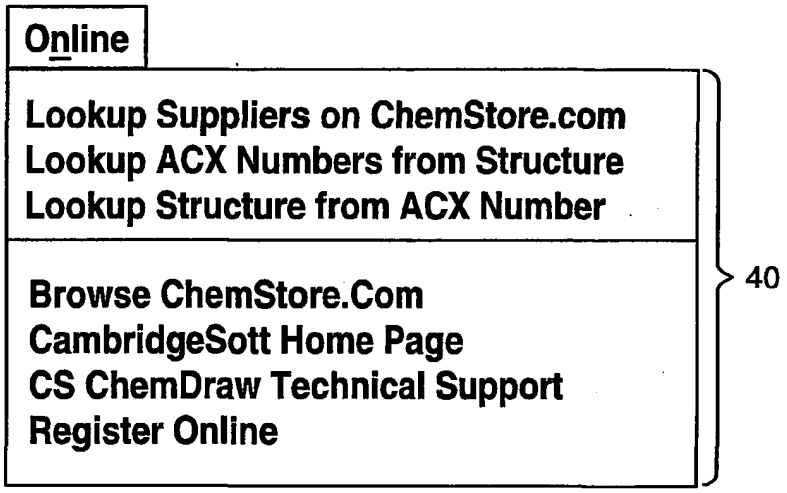

Online
Lookup Suppliers on ChemStore.com
Lookup ACX Numbers from Structure
Lookup Structure from ACX Number
Browse ChemStore.Com
CambridgeSott Home Page
CS ChemDraw Technical Support
Register Online
40

FIG. 3

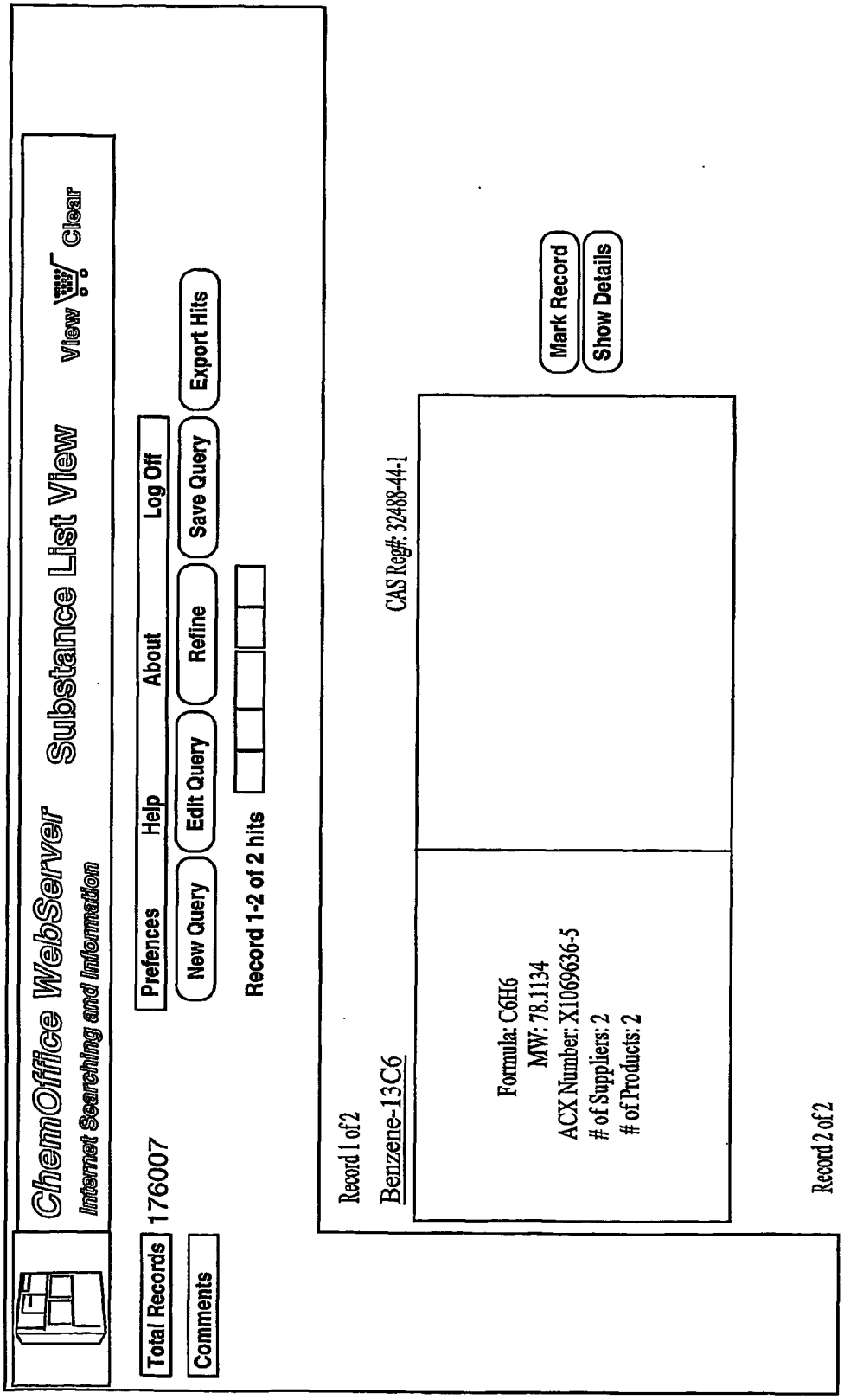

ChemOffice WebServer
Internet Searching and Information
Substance List View
View
Clear
Total Records 176007
Comments
Prefences
Help
About
Log Off
New Query
Edit Query
Refine
Save Query
Export Hits
Record 1-2 of 2 hits
Record 1 of 2
Benzene-13C6
CAS Reg#: 32488-44-1
Formula: C6H6
MW: 78.1134
ACX Number: X1069636-5
# of Suppliers: 2
# of Products: 2
Mark Record
Show Details
Record 2 of 2

FIG. 4

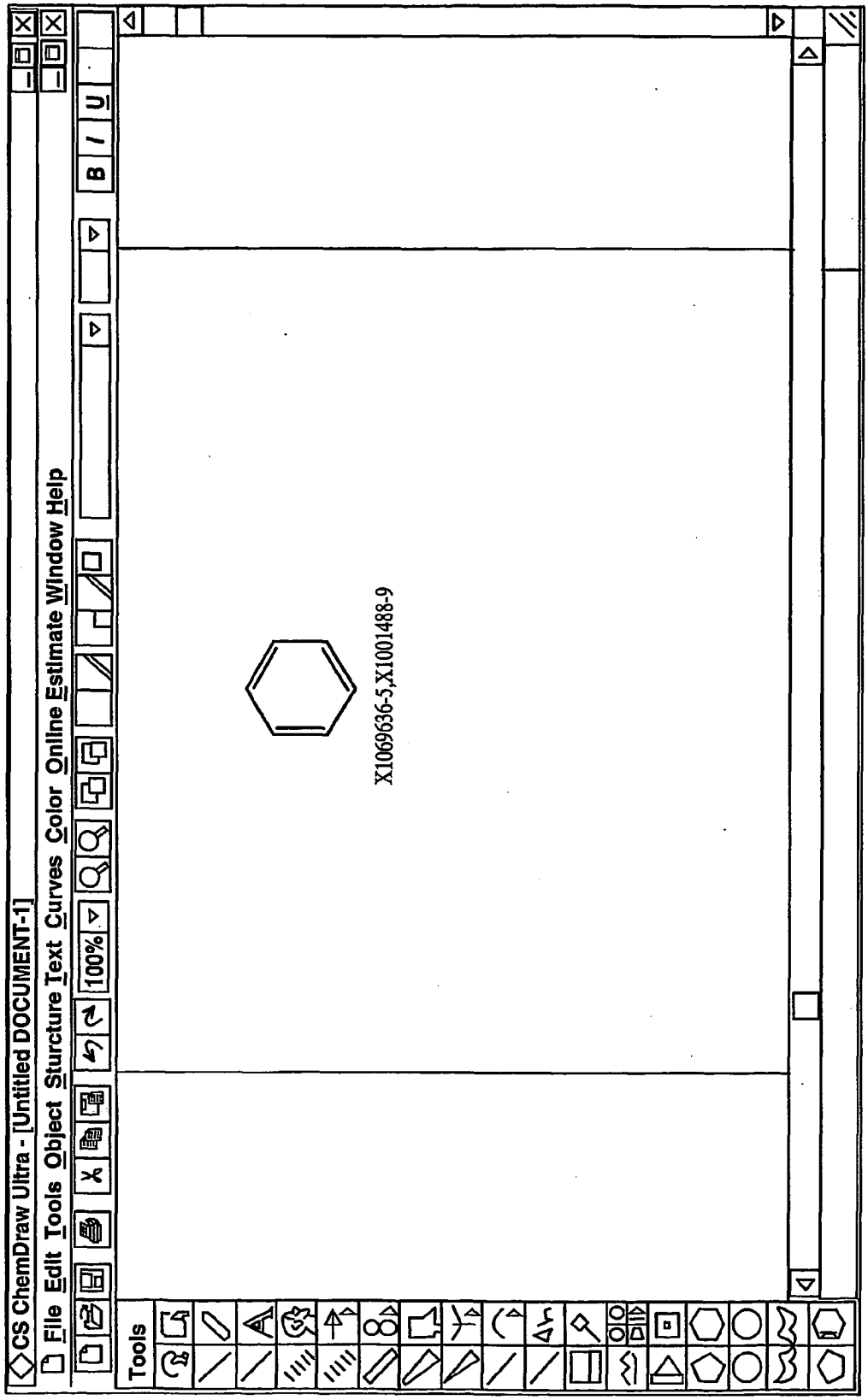

CS ChemDraw Ultra - [Untitled DOCUMENT-1]
File Edit Tools Object Sturcture Text Curves Color Online Estimate Window Help
100%
B I U
Tools
X1069636-5,X1001488-9

FIG. 5

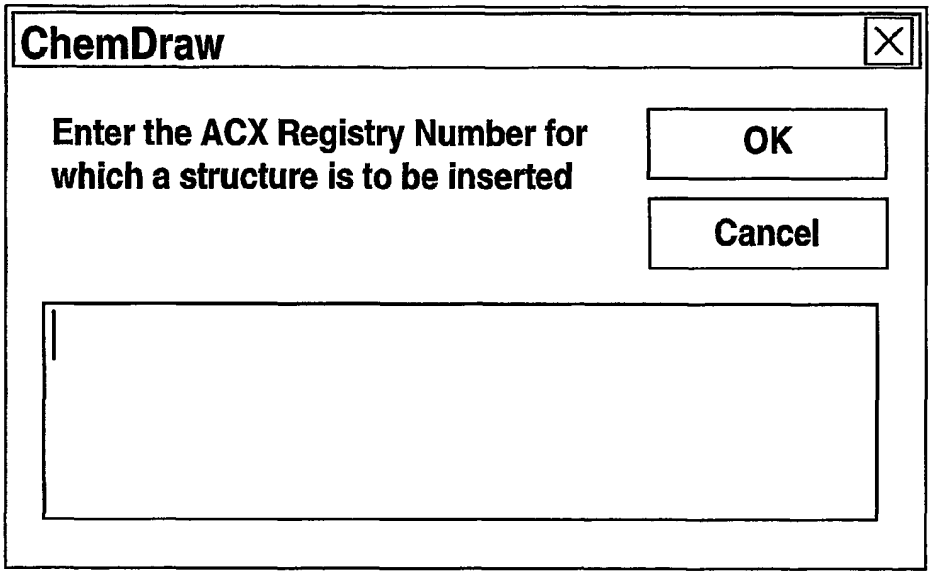

ChemDraw
Enter the ACX Registry Number for which a structure is to be inserted
OK
Cancel

FIG. 6

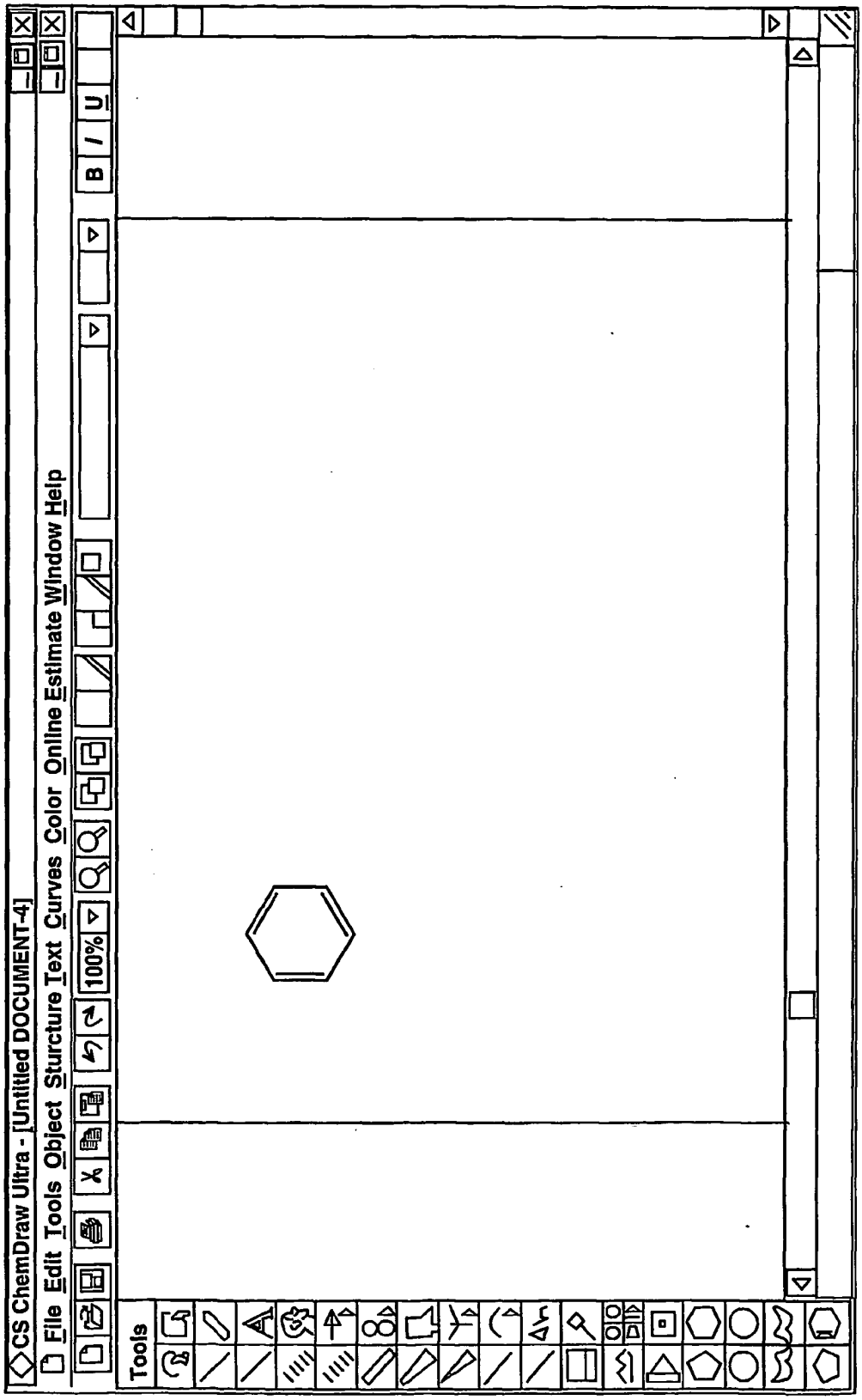
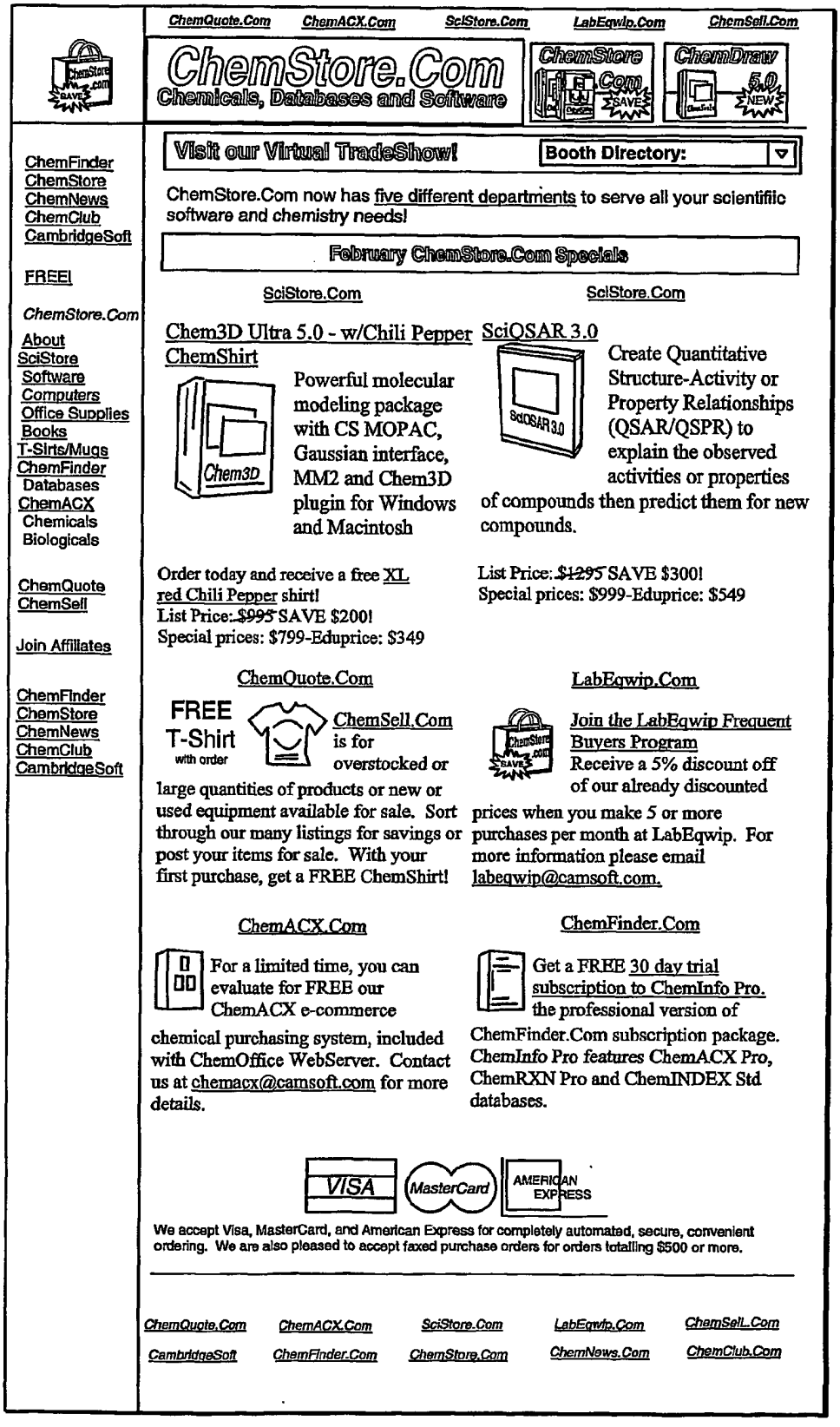

CS ChemDraw Ultra - [Untitled DOCUMENT-4]
File Edit Tools Object Sturcture Text Curves Color Online Estimate Window Help
100%
B I U
Tools

FIG. 7


ChemQuote.Com ChemACX.Com SciStore.Com LabEqwip.Com ChemSell.Com
ChemStore.Com
Chemicals, Databases and Software
ChemStore.Com
ChemDraw 5.0 NEW
ChemFinder
ChemStore
ChemNews
ChemClub
CambridgeSoft
FREE!
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Office Supplies
Books
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ChemFinder Databases
ChemACX Chemicals Biologicals
ChemQuote
ChemSell
Join Affiliates
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ChemNews
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Visit our Virtual TradeShow!
Booth Directory:
ChemStore.Com now has five different departments to serve all your scientific software and chemistry needs!
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Special prices: $999-Eduprice: $549
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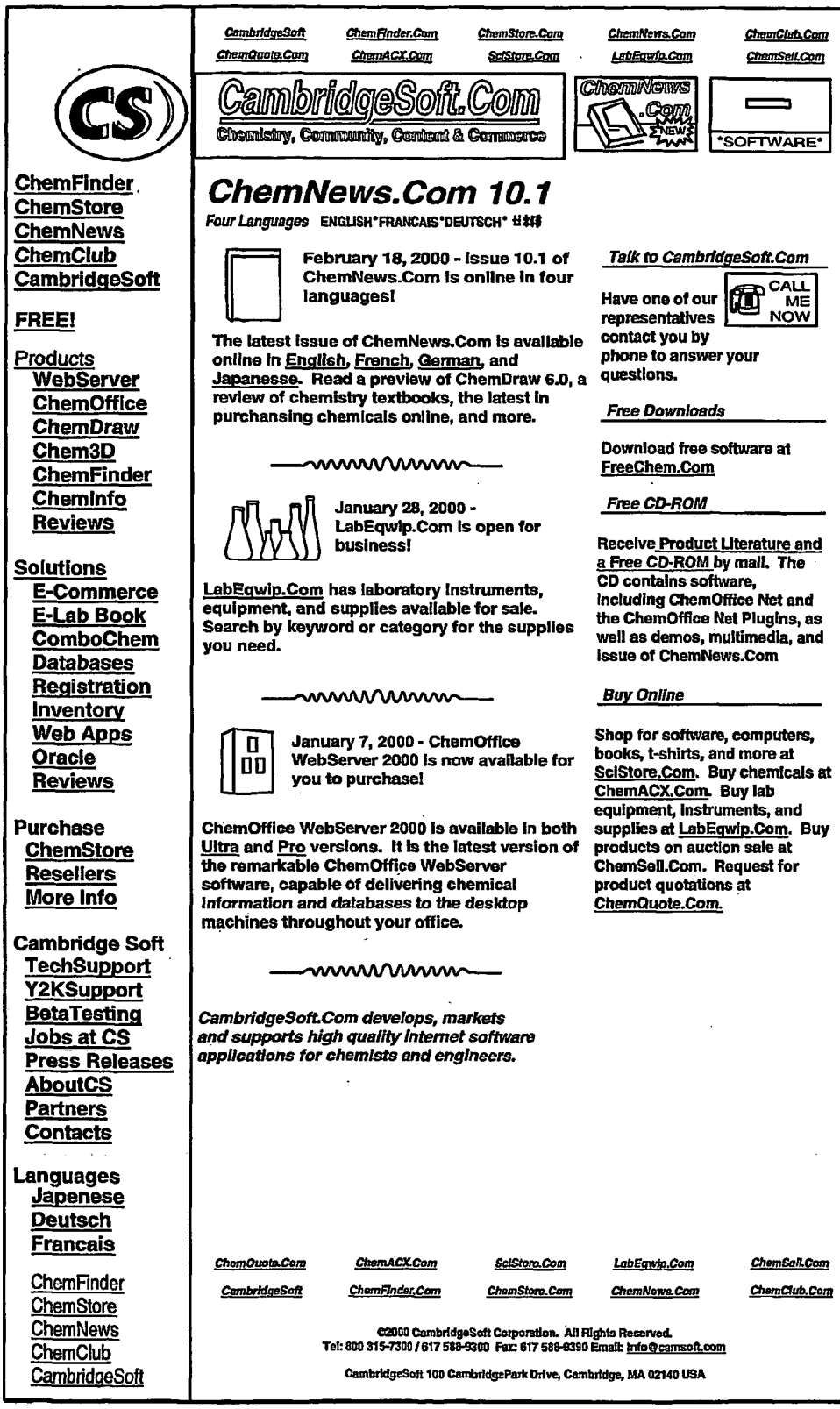
ChemQuote.Com ChemACX.Com SciStore.Com LabEqwip.Com ChemSell.Com
CambridgeSoft ChemFinder.Com ChemStore.Com ChemNews.Com ChemClub.Com

FIG. 8


CambridgeSoft ChemFinder.Com ChemStore.Com ChemNews.Com ChemClub.Com
ChemQuote.Com ChemACX.Com SciStore.Com LabEqwip.Com ChemSell.Com
CambridgeSoft.Com
Chemistry, Community, Content & Commerce
ChemNews.Com
SOFTWARE
ChemFinder
ChemStore
ChemNews
ChemClub
CambridgeSoft
FREE!
Products
WebServer
ChemOffice
ChemDraw
Chem3D
ChemFinder
ChemInfo
Reviews
Solutions
E-Commerce
E-Lab Book
ComboChem
Databases
Registration
Inventory
Web Apps
Oracle
Reviews
Purchase
ChemStore
Resellers
More Info
Cambridge Soft
TechSupport
Y2KSupport
BetaTesting
Jobs at CS
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AboutCS
Partners
Contacts
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Deutsch
Francais
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CambridgeSoft 100 CambridgePark Drive, Cambridge, MA 02140 USA

FIG. 9

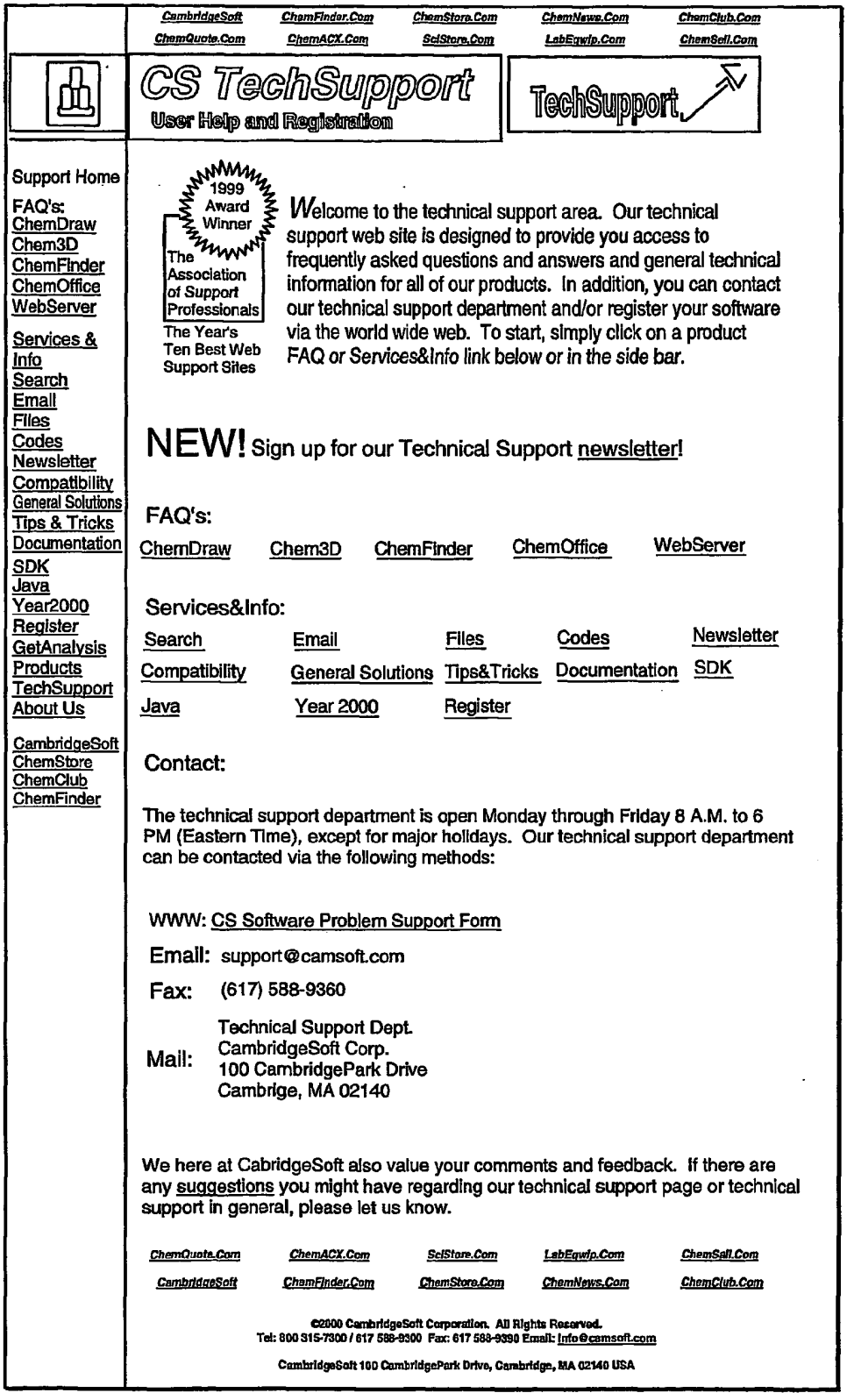
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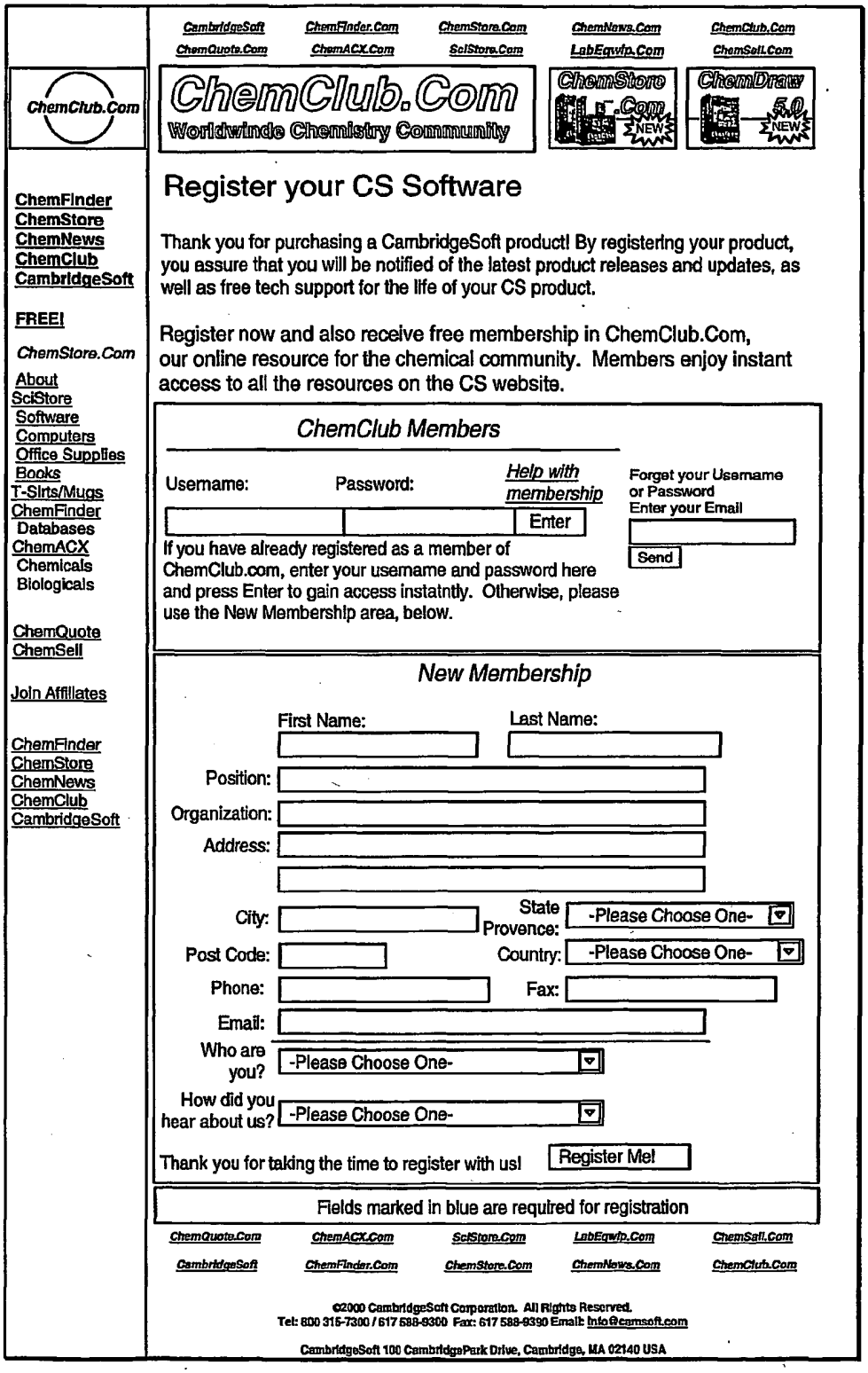
FIG. 10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ChemQuote.Com ChemACX.Com SciStore.Com LabEqwip.Com ChemSell.Com
ChemClub.Com
ChemClub.Com
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FIG. 11

```
01983569  56 6A 43 44 30 31 30 30 04 03 02 01 00 00 00 00 00 00  VjCD0100........
01983579  00 00 00 00 00 00 00 00 00 00 00 00 00 03 00 12 00 00  ................
01983589  00 00 43 68 65 6D 44 72 61 77 20 36 2E 30 2E 33 33  ..ChemDraw 6.0.3
```

FIG. 12A-1

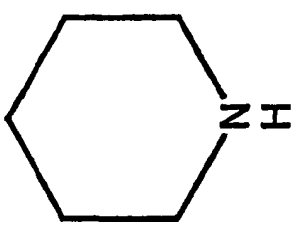

FIG. 12A

FIG. 12A-1	FIG. 12A-2	FIG. 12A-3

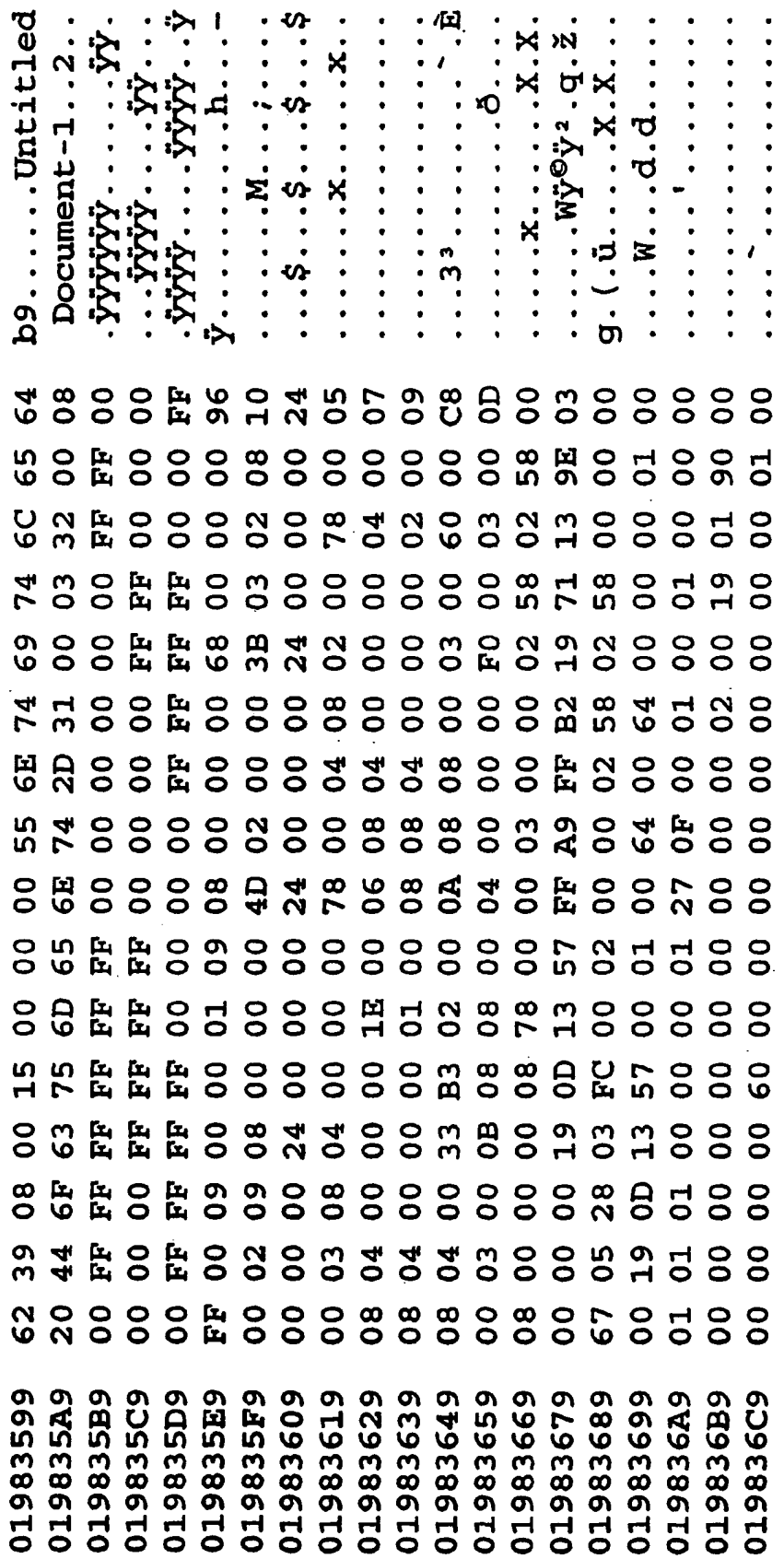
01983599 62 39 08 00 15 00 00 00 55 6E 74 69 74 6C 65 64 b9.....Untitled
019835A9 20 44 6F 63 75 6D 65 6E 74 2D 31 00 03 32 00 08 Document-1..2..
019835B9 00 FF FF FF FF FF 00 00 00 00 00 00 FF FF 00 00 ÿÿÿÿÿÿ.....ÿÿ..
019835C9 00 00 00 FF FF FF 00 00 00 00 FF FF 00 00 00 00 ...ÿÿÿ.....ÿÿ....
019835D9 00 FF FF FF FF FF 00 00 00 00 FF FF FF FF 00 FF .ÿÿÿÿÿ.....ÿÿÿÿ.ÿ
019835E9 FF 00 09 00 00 01 09 08 00 00 00 68 00 00 00 96 ÿ.........h...-
019835F9 00 02 09 08 00 00 00 4D 02 00 00 3B 03 02 08 10 ....M...;....
01983609 00 00 00 24 00 00 00 24 00 00 00 24 00 00 00 24 ...$.....$.....$
01983619 00 03 08 04 00 00 00 78 00 04 08 02 00 78 00 05 ....x.....x..
01983629 08 04 00 00 00 1E 00 06 08 04 00 00 00 04 00 07 ....
01983639 08 04 00 00 00 01 00 08 08 04 00 00 00 02 00 09 ....
01983649 08 04 00 33 B3 02 00 0A 08 08 00 03 00 60 00 C8 ...3³.........`.È
01983659 00 03 00 0B 08 08 00 04 00 00 00 F0 00 03 00 0D ....ð....
01983669 08 00 00 00 08 78 00 00 03 00 00 02 58 02 58 00 .....x.....X.X.
01983679 00 00 00 19 0D 13 57 FF A9 FF B2 19 71 13 9E 03 ......Wÿ©ÿ².q.ž.
01983689 67 05 28 03 FC 00 02 00 00 02 58 02 58 00 00 00 g.(.ü.....X.X...
01983699 00 19 0D 13 57 00 01 00 64 00 64 00 00 00 01 00 ....W...d.d.....
019836A9 01 01 01 00 00 00 01 27 0F 00 01 00 01 00 00 00 ....'........
019836B9 00 00 00 00 00 00 00 00 00 00 02 00 19 01 90 00 ....
019836C9 00 00 00 00 60 00 00 00 00 00 00 00 00 00 01 00 ....`...........

FIG. 12A-2

```
019836D9  00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 04  ................
019836E9  02 10 00 00 00 5E 00 00 00 BD 00 00 00 00 AE 00  .....^.....½...®..
019836F9  00 FA 00 00 01 24 00 00 00 02 00 03 00 E4 04 05  .ú...$.......ä..
01983709  00 41 72 69 61 6C 04 00 E4 04 0F 00 54 69 69 6D  .Arial..ä...Time
01983719  73 20 4E 65 77 20 52 6F 6D 61 6E 01 80 0E 00 00  s New Roman.€...
01983729  00 04 02 10 00 00 5E 00 00 00 BD 00 00 00 AE 00  ......^....½...®.
01983739  00 00 00 FA 00 0F 08 02 00 01 00 10 08 02 00 01  ...ú.............
01983749  00 16 08 04 00 00 24 00 18 08 04 00 00 00 24 00  ......$.......$.
01983759  00 19 08 00 00 03 80 0F 00 00 00 04 02 10 00 00  .....€..........
01983769  00 60 00 00 00 BF 00 00 00 AC 00 00 00 F8 00 04  .`...¿...¬...ø..
01983779  80 01 00 00 00 0A 00 02 00 01 00 00 02 08 00 00  €...............
01983789  00 71 00 EC 04 C1 00 37 04 01 00 01 00 00 04 80  .q.ì.Á.7.......€
01983799  02 00 00 00 0A 00 02 00 02 00 00 02 08 00 00 00  ................
019837A9  8F 00 EC 04 C1 00 37 04 01 00 01 00 00 04 80 03  ..ì.Á.7.......€.
019837B9  00 00 00 0A 00 02 00 03 00 00 02 08 00 00 00 9E  ...............ž
019837C9  00 00 00 DB 00 06 80 0D 00 00 00 0A 00 02 00 0D  ...Û..€.........
019837D9  00 00 00 07 0E 00 01 00 00 00 03 00 60 00 C8 00  ............`.È..
019837E9  00 4E 48 04 07 06 00 02 00 02 00 03 00 05 07 01  .NH.............
019837F9  00 05 00 02 08 00 66 E6 A1 00 00 30 D8 00 04 02  ......fæ¡..0Ø...
01983809  10 00 00 00 9B 00 00 00 D9 00 00 00 AC 00 00 00  ....›...Ù...¬...
01983819  DE 00 00 00 37 04 01 00 01 02 04 02 00 07 00 2B  Þ...7..........+
01983829  04 02 00 01 00 00 00 04 80 04 00 00 00 0A 00 02  .........€......
```

FIG. 12A-3

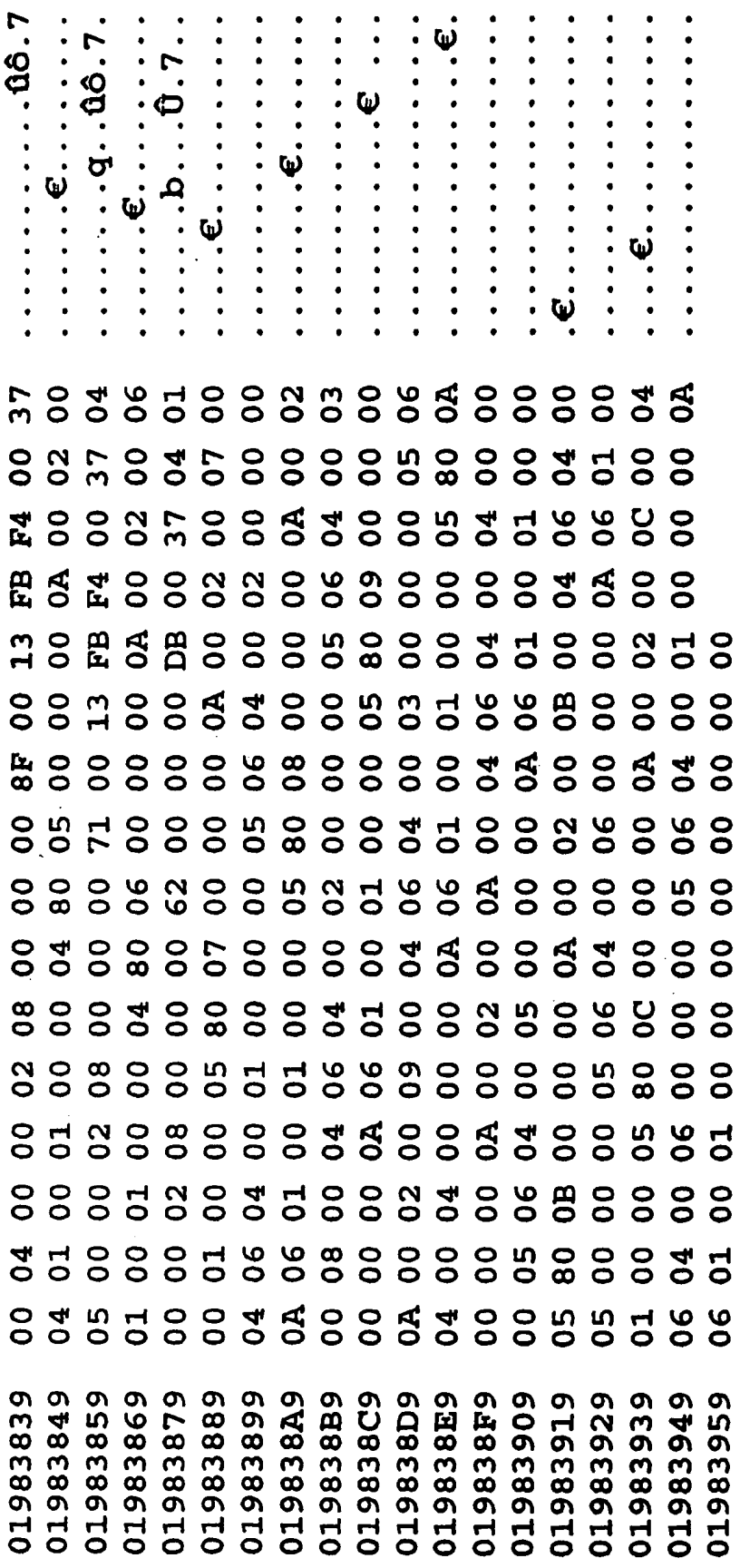
01983839 00 04 00 00 02 08 00 00 8F 00 13 FB F4 00 37 .....ûô.7
01983849 04 01 00 01 00 00 04 80 05 00 00 00 0A 00 02 00 .....€.....
01983859 05 00 00 00 02 08 00 00 00 71 00 13 FB F4 00 37 04 .....q..ûô.7.
01983869 01 00 01 00 00 00 04 80 06 00 00 00 0A 00 02 00 06 .....€.....
01983879 00 00 02 08 00 00 00 62 00 00 00 00 DB 00 37 04 01 .....b....Û.7..
01983889 00 01 00 00 00 05 80 07 00 00 00 0A 00 02 00 07 00 ....€.....
01983899 04 06 04 00 01 00 00 00 05 06 04 00 02 00 00 00 00 .....
019838A9 0A 06 01 00 01 00 00 05 80 08 00 00 00 0A 00 02 .....€.....
019838B9 00 08 00 04 06 04 00 02 00 00 00 05 06 04 00 03 .....
019838C9 00 00 00 0A 06 01 00 01 00 00 05 80 09 00 00 00 .....€ ...
019838D9 0A 00 02 00 09 00 04 06 04 00 03 00 00 00 05 06 .....
019838E9 04 00 04 00 00 00 0A 06 01 00 01 00 00 05 80 0A .....€.
019838F9 00 00 00 0A 00 02 00 0A 00 04 06 04 00 04 00 00 .....
01983909 00 05 06 04 00 05 00 00 00 0A 06 01 00 01 00 00 .....
01983919 05 80 0B 00 00 00 0A 00 02 00 0B 00 04 06 04 00 .€.....
01983929 05 00 00 00 00 05 06 04 00 06 00 00 00 0A 06 01 00 .....
01983939 01 00 00 00 05 80 0C 00 00 00 0A 00 02 00 0C 00 04 ....€.....
01983949 06 04 00 06 00 00 00 05 06 04 00 01 00 00 00 0A .....
01983959 06 01 00 01 00 00 00 00 00 00 00 00 00 00 00 00

FIG. 12B

VmpDRDAxMDAEAwIBAAAAAAAAAAAAAAAAAMAEgAAAENoZW1EcmF3IDYuMC4z
YjkIABUAAABVbnRpdGx1ZCBEb2N1bWVudC0xAAMyAAgA//////////AAAAAAAA//8A
AAAA/////wAAAAD/////AAAAAP////8AAP//AAkAAAEJCAAAAGgAAACW
AAIJCAAAAE0CAAA7AwIIEAAAACQAAAAkAAAAJAAAACQAAwgEAAAAeAAECAIAeAAF
CAQAAAAeAAYIBAAAAAQABwgEAAAAAQAICAQAAAACAAkIBAAzswIACggIAAMAYADI
AAMACwgIAAQAAADwAAMADQgAAAAIeAAAAwAAA1gCWAAAAAAAZDRNX/6n/sh1xE54D
ZwUoA/wAAgAAA1gCWAAAAAAZDRNXAAEAZABkAAAAAAQABAQEAAAABJw8AAQABAAAA
AAAAAAAAAAAAAAAAAAIAGQGQAAAAAAABgAAAAAAAAAAAQAAAAAAAAAAAAAAAAAE
AhAAAABeAAAAvQAAAK4AAAD6AAABJAAAAAIAAwDkBAUAQXJpYWwEAOQEDwBUaW11
cyBOZXcgUm9tYW4BgA4AAAAEAhAAAABeAAAAvQAAAK4AAAD6AA8IAgABAAIAgAB
ABYIBAAAACQAGAgEAAAAJAAZCAAAA4APAAABAIQAAAAYAAAAL8AAACsAAAA+AAE
gAEAAAAKAAIAAQAAAggAAABxAOwEwQA3BAEAAQAABIACAAAACgACAAIAAAIIAAAA
jwDsBMEANwQBAAEAAASAAwAAAAoAAgADAAACCAAAAJ4AAADbAAaADQAAAAoAAgAN
AAAHDgABAAAAAAwBgAMgAAwBOSAQHBgACAAIAAwAFBwEABQACCABm5qEAADDYAAQC
EAAAAJsAAADZAAAArAAAN4AAAA3BAEAAQIEAgAHACsEAgABAAAABIAEAAAACgAC
AAQAAAIIAAAAjwAT+/QANwQBAAEAAASABQAAAAoAAgAFAAACCAAAAHEAE/v0ADcE
AQABAAAEgAYAAAAKAAIABgAAAggAAABiAAAA2wA3BAEAAQAABYAHAAAACgACAAcA
BAYEAAEAAAAAFBgQAAgAAAAoGAQABAAAAFgAgAAAAKAAIACAAEBgQAAgAAAAUGBAAD
AAAACgYBAAEAAAWACQAAAAoAAgAJAAQGBAADAAAABQYEAAQAAAKBgEAAQAABYAK
AAAACgACAAoABAYEAAQAAAAFBgQABQAAAAoGAQABAAAFgAsAAAAKAAIACwAEBgQA
BQAAAAUGBAAGAAAACgYBAAEAAAWADAAAAAoAAgAMAAQGBAAGAAAABQYEAAEAAAAK
BgEAAQAAAAAAAAA

FIG. 13

FIG. 14A
FIG. 14B

FIG. 14

```
POST HTTP/1.1
/chemacx/chemacx_action.asp?dbname=chemacx&dataaction=search_no_gui
Accept: */*
Host: chemdraw.chemacx.com
Referer: Online
User-Agent: CS ChemDraw Ultra 6.0
Cookie: ASPSESSIONIDGGGGGRTD=BELBBHJCLDCFHMOPNDDKFLBO
Content-Length: 1481
Content-Type: application/x-www-form-urlencoded
Cache-Control: no-cache
```

FIG. 14A

```
return_fields=Substance.ACX_ID&struc_search_type=exact&Substance.Structure=
VmpDRDAxMDAEAwIBAAAAAAAAAAAAAAAAAAAAAAMAEgAAAENoZW1EcmF3IDYuMC4z
YjkIABUAAAABVbnRpdGx1ZCBEb2N1bWVudC0xAAMyYAAgA/////////AAAAAAAA//8A
AAAA/////wAAAAD//////AAAAAP////8AAP//AAkAAAAEJCAAAAGgAAACW
AAIJCAAAAE0CAAA7AwIIEAAAACQAAAkAAAAJAAAACQAAwgEAAAAeAAECAIAeAAF
CAQAAAAeAAYIBAAAAAQABwgEAAAAAQAICAQAAAACAAkIBAAzswIACggIAAMAYADI
AAMACwgIAAQAAADwAAMADQgAAAAIeAAAAwAAAlgCWAAAAAAAZDRNX/6n/sh1xE54D
ZwUoA/wAAgAAA1gCWAAAAAAZDRNXAAEAZABkAAAAAAQABAQEAAAABJw8AAQABAAAA
AAAAAAAAAAAAAAAAIAGQGQAAAAAABgAAAAAAAAAAAAQAAAAAAAAAAAAAAAAAAE
AhAAAABeAAAAvQAAAK4AAAD6AAABJAAAAAIAAwDkBAUAQXJpYWwEAOQEDwBUaW11
cyBOZXcgUm9tYW4BgA4AAAAEAhAAAABeAAAAvQAAAK4AAAD6AA8IAgABABAIAgAB
ABYIBAAAACQAGAgEAAAAJAAZCAAAA4APAAAABAIQAAAAYAAAAL8AAACsAAAA%2bAAE
gAEAAAAKAAIAAQAAAggAAABxAOwEwQA3BAEAAQAABIACAAAACgACAAIAAAIIAAAA
jwDsBMEANwQBAAEAAASAAwAAAAoAAgADAAACCAAAAJ4AAADbAAaADQAAAAoAAgAN
AAAHDgABAAAAAAwBgAMgAAwBOSAQHBgACAAIAAwAFBwEABQACCABm5qEAADDYAAQC
EAAAAJsAAADZAAAArAAAN4AAAA3BAEAAQIEAgAHACsEAgABAAAABIAEAAAACgAC
AAQAAAIIAAAAjwAT%2b/QANwQBAAEAAASABQAAAAoAAgAFAAACCAAAAHEAE/v0ADcE
AQABAAAEgAYAAAAKAAIABgAAAggAAABiAAAA2wA3BAEAAQAABYAHAAAACgACAAcA
BAYEAAEAAAAAFBgQAAgAAAAoGAQABAAAFgAgAAAAKAAIACAAEBgQAAgAAAAUGBAAD
AAAACgYBAAEAAAWACQAAAAoAAgAJAAQGBAADAAAABQYEAAQAAAAKBgEAAQAABYAK
AAAACgACAAoABAYEAAQAAAAFBgQABQAAAAoGAQABAAAFgAsAAAAKAAIACwAEBgQA
BQAAAAUGBAAGAAAAACgYBAAEAAAWADAAAAAoAAgAMAAQGBAAGAAAABQYEAAEAAAAK
BgEAAQAAAAAAAAAA
```

FIG. 14B

```
HTTP/1.1 200 OK
Server: Microsoft-IIS/4.0
Date: Wed, 28 Feb 2001 17:34:38 GMT
Content-Type: text/html
Cache-control: private
Transfer-Encoding: chunked

X1001495-4
```

FIG. 15

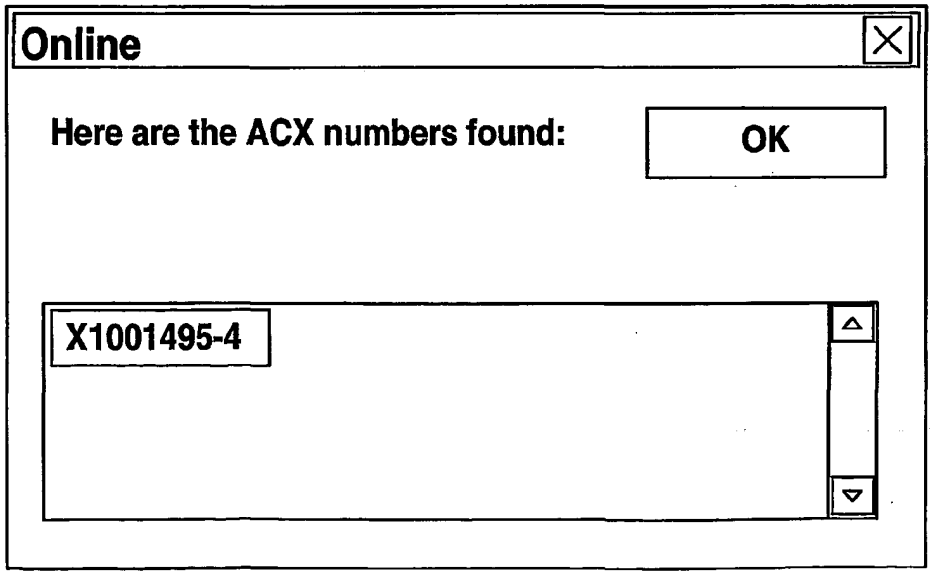

FIG. 16

INTERNATIONAL SEARCH REPORT

Internati pplication No
PCT/US 01/06443

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 G06F17/30

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

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C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	IHLENFELDT W-D ET AL: "BEYOND THE HYPERACTIVE MOLECULE: SEARCH, SALVAGE AND VISUALIZATION OF CHEMICAL INFORMATION FROM THE INTERNET" PACIFIC SYMPOSIUM ON BIOCOMPUTING '96. HAWAII, JAN. 3 - 6, 1996, SINGAPORE, WORLD SCIENTIFIC, SI, vol. SYMP. 1, 3 January 1996 (1996-01-03), pages 384-395, XP000751937 ISBN: 981-02-2578-4 section 4: Application Examples figures 1-5 --- -/—	1-14

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Date of the actual completion of the international search	Date of mailing of the international search report
27 June 2002	04/07/2002

Name and mailing address of the ISA	Authorized officer
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X	ERTL P ET AL: "WWW-BASED CHEMICAL INFORMATION SYSTEM" JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM), ELSEVIER SCIENCE PUBLISHERS B.V., AMSTERDAM, NL, vol. 419, 8 December 1997 (1997-12-08), pages 113-120, XP000957419 ISSN: 0166-1280 Section 1: Introduction figures 1-7 ---	1-14
A	US 5 978 804 A (DIETZMAN GREGG R) 2 November 1999 (1999-11-02) column 2, line 64 -column 3, line 67 ---	1,13,14
A	US 6 023 659 A (AKERBLOM INGRID E ET AL) 8 February 2000 (2000-02-08) column 2, line 16 -column 4, line 20 -----	1,13,14

INTERNATIONAL SEARCH REPORT

Information on patent family members

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PCT/US 01/06443

Patent document cited in search report		Publication date	Patent family member(s)		Publication date
US 5978804	A	02-11-1999	NONE		
US 6023659	A	08-02-2000	US	6363399 B1	26-03-2002
			US	5953727 A	14-09-1999
			US	6189013 B1	13-02-2001